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Adsorption of Energy-Related Organic Pollutants

A Literature Review

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This report is a literature review on sorption properties of sediments and energy-related organic pollutants. Adsorption of organic compounds in general is discussed, and analytical methodology in soil thin-layer chromatography and chemical analysis as applicable to measurement of sorption properties is summarized. The literature on the adsorption of energy-related organic pollutants is reviewed. Reported constants for the adsorption of organic compounds on several adsorbents are tabulated, and factors that influence adsorption are discussed.

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ADSORPTION OF ENERGY-RELATED ORGANIC POLLUTANTS: A LITERATURE REVIEW

by

K. A. Reinbold, J. J. Hassett,
J. C. Means, and W. L. Banwart
Institute for Environmental Studies
and
Department of Agronomy
University of Illinois at Urbana-Champaign
Urbana, Illinois 61801

Contract No. 68-03-2555

Project Officer

David S. Brown
Environmental Processes Branch
Environmental Research Laboratory
Athens, Georgia 30605

ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ATHENS, GEORGIA 30605

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FOREWORD

Environmental protection efforts are increasingly directed towards prevention of adverse health and ecological effects associated with specific compounds of natural or human origin. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Environmental Processes Branch studies the microbiological, chemical, and physico-chemical processes that control the transport, transformation, and impact of pollutants in soil and water.

Efforts to achieve our national goal of energy independence will require increasing use of our country's vast domestic coal reserves. The combustion of coal or its conversion to a gaseous or liquid fuel, however, can release numerous organic compounds that are potentially toxic, carcinogenic, or mutagenic. This report reviews the literature on the adsorption of energy-related organic pollutants and other compounds on sediments and soils. Information on the adsorption of these pollutants onto sediments is needed to predict their movement and fate in aquatic systems so that potential environmental problems can be anticipated.

David W. Duttweiler
Director
Environmental Research Laboratory
Athens, Georgia

ABSTRACT

This report is a literature review which was completed as the first phase of a research project on sorption properties of sediments and energy-related organic pollutants. Adsorption of organic compounds in general is discussed, and analytical methodology in soil thin-layer chromatography and chemical analysis as applicable to measurement of sorption properties is summarized. The literature on the adsorption of energy-related organic pollutants is reviewed. Reported constants for the adsorption of organic compounds on several adsorbents are tabulated, and factors which influence the adsorption are discussed.

This report was submitted in partial fulfillment of Contract No. 68-03-2555 by the University of Illinois Institute for Environmental Studies in cooperation with the Department of Agronomy under the sponsorship of the U.S. Environmental Protection Agency. This report covers the period of July 1977 to April 1978, and work was completed as of June 1979.

CONTENTS

FOREWORD iii

ABSTRACT iv

FIGURE vi

TABLES vi

ACKNOWLEDGMENTS vii

1. INTRODUCTION 1

2. SUMMARY AND CONCLUSIONS 8

3. ADSORPTION OF ORGANIC COMPOUNDS 9

   The Solid-Solution Interface 9
   Adsorptive Forces 9
   Adsorption Isotherms 11

4. ANALYTICAL PROCEDURES: SOIL THIN-LAYER CHROMATOGRAPHY 18

5. ANALYTICAL PROCEDURES: CHEMICAL ANALYSIS 22

   Recovery of Organic Compounds from Environmental Samples 22
   Fractionation, Cleanup, and Separation of Organic Extract Components 23
   Quantitation of Trace Organic Compounds in Solvent Extracts 24

6. REVIEW AND INTERPRETATION OF ADSORPTION DATA 30

   Factors Influencing Adsorption 30
   Interpretation of Tabulated Data 34

BIBLIOGRAPHY 114

   Adsorption of Organic Compounds 114
   Analytical Procedures 134
   Compound Characteristics 153
   Occurrence and Distribution of Energy-related Organic Compounds 158

APPENDIX: FORMULAS OF ORGANIC COMPOUNDS 161

FIGURE

1. Functional Group Model of Bituminous Coal 2

TABLES

1. Organic Contaminants Present in Coal Tar from the Synthane Coal Conversion Process 3
2. Contaminants Present in Product Water from the Gasification of Illinois No. 6 Coal 4
3. Classes of Known or Suspected Carcinogenic or Cocarcinogenic Compounds Associated with Processing and Utilization of Coal 5
4. Selected Energy-Related Organic Compounds 7
5. Kow, Calculated Koc, Linear Kp and Measured Koc Values for Sorption of Pyrene, Dibenzothiophene and Acetophenone by Soils and Sediments 33
6. Adsorption Constants for Organic Compounds 36
7. Average Values of Adsorption Constants for Organic Pesticides 89
8. Relationship between Octanol/Water Partition and R_f Values of Pesticides on a Soil 107
9. Leaching of Pesticides from a Soil 108
10. Sorption Dependence on Sorbate Properties 109

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The literature review presented in this report was conducted under the direction of Dr. Keturah A. Reinbold, associate research biologist, with the assistance of Ms. Dee Condon and Ms. Carol Wells, research assistants, in conducting the literature search. Information on soil thin-layer chromatography was summarized by Dr. Wayne L. Banwart, assistant professor of soils. Appreciation is expressed to Thomas Knecht, publications director of the Institute for Environmental Studies, and Cindy Bohde, student editorial assistant, for the technical editing of this report and to Jean Clarke, Judith Jones, Trace Black, and Sharon Sparling for typing the report.

1 INTRODUCTION

Fossil fuels are a major source of anthropogenic organic compounds in the environment. Because supplies of petroleum and natural gas are dwindling, it will be necessary to utilize increasing amounts of coal to meet our energy needs in the near future. As Figure 1 illustrates, coal is a complex organic chemical. Either the combustion of coal or its conversion to a gaseous or liquid fuel breaks the coal into numerous simpler organic compounds, which then appear in process waste streams and may be released into the environment. These coal fragments include a great variety of polycyclic aromatics, heterocyclic- and carbonyl-polycyclics, and aromatic amines, groups which all contain known or suspected carcinogens, as well as phenolics and long-chain aliphatic hydrocarbons (TRW Systems and Energy, 1976; Sharkey *et al.*, 1976).

Coal conversion processes produce large volumes of gaseous and aqueous effluents (Magee, Bertrand, and Jahnig, 1976). Hundreds of thousands of tons of gases containing volatile organics, particulates, and combustion gases are released each day. These emissions may disperse over hundreds of miles, distributing the effluent materials in both terrestrial and aquatic systems. With such large volumes of effluents, even trace components are distributed in significant amounts--up to hundreds of pounds per year. Some of these materials are potentially toxic, carcinogenic, or mutagenic.

Aqueous effluents may be released at a rate of up to 5 million gallons each day. Also, large volumes of aqueous leachate from stockpiles of coal or solid wastes, such as ash and char, are produced. The wastes from the various steps of the coal conversion process contain a variety of organic materials.

A number of organic products have been detected in the wastes from coal conversion pilot plants. Forney *et al.* (1974) identified some of the major organic compounds in tars produced by the Synthane coal gasification process (Table 1), and Schmidt, Sharkey, and Friedel (1974) analyzed the process water (Table 2). TRW Systems and Energy (1976) listed several organic compounds which are associated with the processing and utilization of coal and which are known or suspected carcinogenic or cocarcinogenic compounds (Table 3).

Clearly, large quantities of organic compounds are introduced into aquatic systems, either directly in aqueous effluents or indirectly from gaseous effluents. The behavior of these compounds in aquatic systems depends largely upon the extent to which they are adsorbed on suspended or settled sediments.

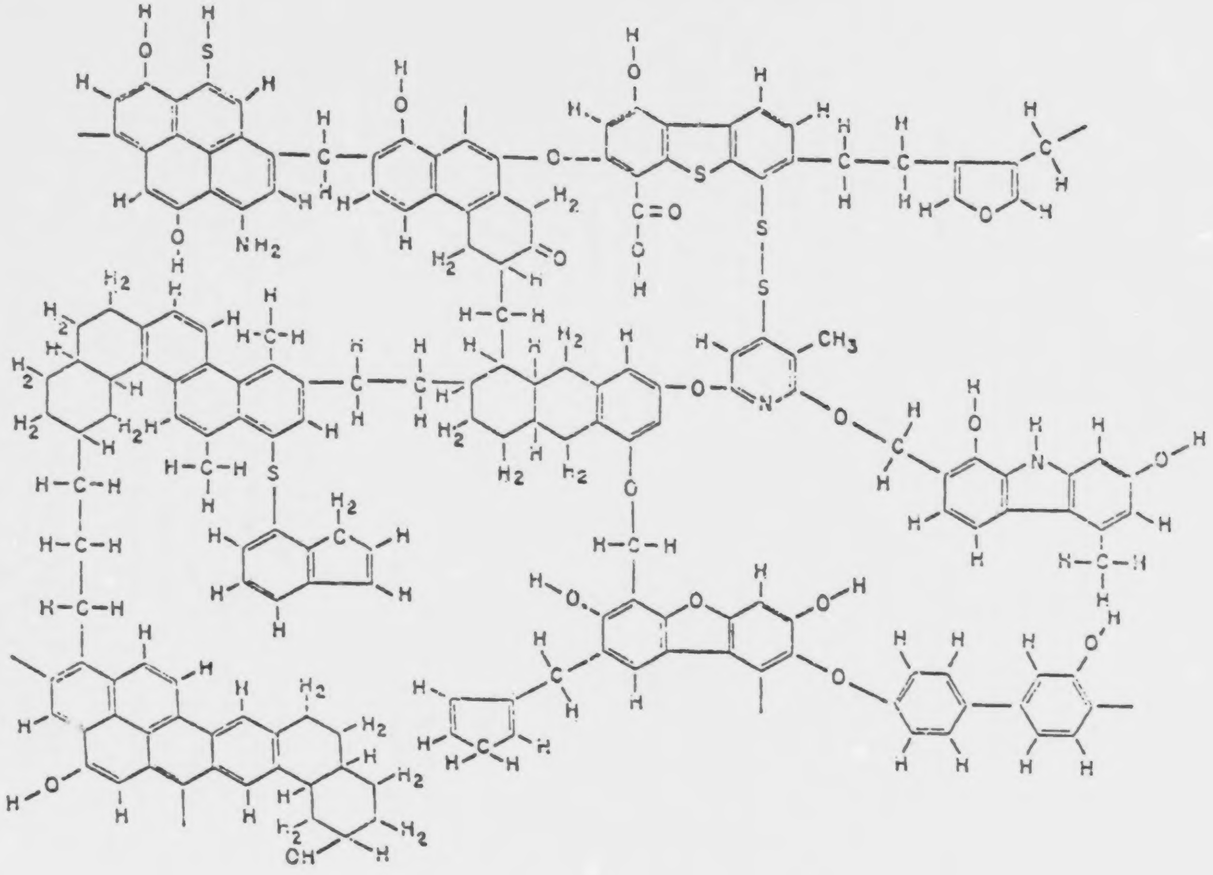


Figure 1. Functional group model of bituminous coal (Wiser).

Source: Wewerka, Williams, and Vanderborgh, 1976.

TABLE 1. ORGANIC CONTAMINANTS PRESENT IN COAL TAR FROM THE SYNTHANE COAL CONVERSION PROCESS

Structural Type	Volume (percent)			
	Illinois No. 6	Lignite	Montana Subbituminous	Pittsburg Seam
Benzenes	2.1	4.1	3.9	1.9
Indenes	8.6	1.5	2.6	6.1
Indanes	1.9	3.5	4.9	2.1
Naphthalenes	11.6	19.0	15.3	16.5
Fluorenes	9.6	7.2	9.7	10.7
Acenaphthenes	13.5	12.0	11.1	15.8
3-ring aromatics	13.8	10.5	9.0	14.8
Phenyl naphthalenes	9.8	3.5	6.4	7.6
4-ring aromatics - peri	7.2	3.5	4.9	7.6
4-ring aromatics - cata	4.0	1.4	3.0	4.1
Phenols	2.8	13.7	5.5	3.0
Naphthols	+	9.7	9.6	+
Indanols	0.9	1.7	1.5	0.7
Acenaphthols	-	2.5	4.6	2.0
Phenanthrols	2.7	-	0.9	-
Dibenzofurans	6.3	5.2	5.6	4.7
Dibenzothiophenes	3.5	1.0	1.5	2.4
Benzonaphthothiophenes	1.7	-	-	-
N-heterocycles	10.8	3.8	5.3	8.8

Source: Forney *et al.*, 1974

TABLE 2. CONTAMINANTS PRESENT IN PRODUCT WATER FROM THE GASIFICATION OF ILLINOIS NO. 6 COAL

Compound	Concentration (ppm)
Phenols	2,660 to 3,400
Cresols	2,610 to 2,840
C_2-phenols	560 to 1,170
C_3-phenols	70 to 150
Dihydric phenols	60 to 300
Benzofuranols	70 to 120
Indanols	60 to 210
Acetophenones	
Benzoic Acids	
Hydroxybenzaldehyde	40 to 210
Naphthols	110 to 160
Indenols	90
Benzofurans	10 to 30
Dibenzofurans	10
Biphenols	20 to 40
Benzothiophenols	60 to 110
Pyridines	60 to 580
Quinolines	10 to 20
Indoles	20 to 70

Source: Schmidt, Sharkey, and Friedel, 1974.

OBJECTIVES

To examine the adsorption of energy-related organic compounds in the environment, a research project was initiated in the Institute for Environmental Studies at the University of Illinois at Urbana-Champaign. The project is supported by the U.S. Environmental Protection Agency under contract number 68-03-2555. This report presents the results of the first phase of the project, the objective of which was to review published literature on (1) the adsorption of energy-related organic pollutants on sediments, (2) the theory of adsorption, and (3) analytical techniques pertinent to adsorption measurements. Because the literature survey produced only a limited amount of information on the adsorption of energy-related organic compounds, a variety of organic compounds were included in this review to provide a background of information.

APPROACH

The literature was searched by a combination of computer and manual methods. The 1970-77 volumes of *Chemical Abstracts* were searched using-the computerized Bibliographic Retrieval Service System. The key words used were terms such as *adsorption, desorption,* and *sediments* accompanied by the names of compound groups or of specific compounds which may be energy-related organic pollutants, including all those listed in Table 4. Earlier volumes of *Chemical Abstracts* were searched manually, as were pertinent books, series of *Residue Reviews,* current journals, and the 1977 *Weekly Government Abstracts* from the National Technical Information Service.

The computerized search produced more than 900 citations. Copies of approximately one-third of these references were obtained for review. With the addition of those acquired by manual searching, a total of 670 references were obtained for review. A bibliography is included at the end of this report.

TABLE 3. CLASSES OF KNOWN OR SUSPECTED CARCINOGENIC OR COCARCINOGENIC COMPOUNDS ASSOCIATED WITH PROCESSING AND UTILIZATION OF COAL

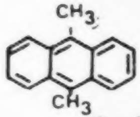
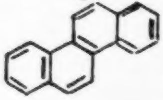
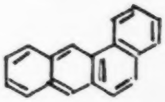
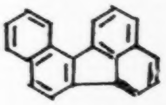
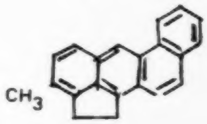
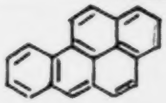
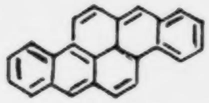
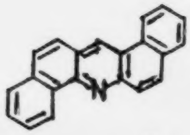
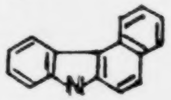
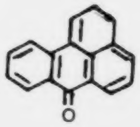
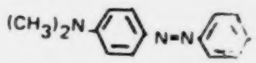
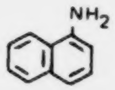
Compound Class	Representative Compound	Structure
Polynuclear Aromatic Hydrocarbons		
Anthracenes	9-,10-dimethylanthracene	
Chrysenes	chrysene	
Benzanthracenes	benzo(a)anthracene	
Fluoranthenes	benzo(j)fluoranthene	
Cholanthrenes	3 -methylcholanthrene	

TABLE 3, *continued*

Compound Class	Representative Compound	Structure
Benzopyrenes	benzo(a)pyrene	
Dibenzpyrenes	dibenzo(a,h)pyrene	
Nitrogen-, Sulfur-, and Oxygen-Containing Polycyclic Compounds		
Mono- and dibenzacridines	dibenz(a,h)acridine	
Benzocarbazoles	7H-benzo(c,g)carbazole	
Benzathrones	7H-benz(d,e)anthracen-7-one	
Aromatic Amines		
Aminoazobenzenes	4-dimethylaminoazobenzene	
Naphthylamines	α-naphthylamine	
Cocarcinogens and Promoting Agents		
Phenols/naphthols	α-naphthol	
Long-chain aliphatic hydrocarbons	n-dodecane	$CH_3-(CH_2)_{10}-CH_3$

Source: TRW Systems and Energy, 1976.

TABLE 4. SELECTED ENERGY-RELATED ORGANIC COMPOUNDS

Polynuclear Aromatics

Anthracene
Phenanthrene
Acenaphthene
Fluorene
Naphthacene
Chrysene
Pyrene
Triphenylene
Perylene
1,2-Benzopyrene
3,4-Benzopyrene
1,2-Benzanthracene
1,2,7,8-Dibenzanthracene
1,2,5,6-Dibenzanthracene
1,2,3,4-Dibenzanthracene
7,12-Dimethylbenzanthracene
3-Methylcholanthrene

S-Heterocyclics

2,3-Benzothiophene
Dibenzothiophene

N-Heterocyclics

Carbazole
Indole
Acridine
Pyridines
Pyrroles
Benzocarbazole
Dibenzocarbazole
Benzoquinoline

Phenolics

1-Naphthol
2-Naphthol
Acenaphthol
4-Indanol
4-Benzofuranol
4-Hydroxybenzothiophene
2,3,4-Trimethyl Phenol

Miscellaneous

Acetophenone
Anthraquinone
Benzidine
Benzophenone

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2 SUMMARY AND CONCLUSIONS

We have reviewed the literature on the adsorption of energy-related organic pollutants and other organic compounds on sediments, soils, and other selected adsorbents. Adsorption constants reported in the literature for organic compounds are compiled in Tables 6 and 7, and factors which influence adsorption are discussed.

Among the many factors which influence adsorption are several molecular properties of compounds. It has been shown that as chain length, molecular volume, molecular weight, and carbon number increase, and as polarity decreases, adsorption of hydrophobic compounds increases. These properties are related to water solubility of the compound. The adsorption of hydrophobic compounds increases with decreasing water solubility, but for more polar compounds adsorption increases with decreasing water solubility only within a family of compounds. Soil organic matter content influences adsorption and has been shown to correlate with the partitioning of nonpolar organic compounds between octanol and water. This relationship makes possible the calculation of Koc and Kp values when Kow is known.

Little of the published information pertains specifically to the adsorption of energy-related organic pollutants onto sediments or soils. Data are available on the adsorption of a few such compounds onto carbon, but those results cannot be directly extrapolated to sediments or soils. Investigation of adsorption of these compounds on sediments is beginning, as in the laboratory phase of this project. Information on the adsorption of these pollutants onto sediments is needed to predict their movement and fate in aquatic systems. To obtain sufficient information, further research is necessary.

3 ADSORPTION OF ORGANIC COMPOUNDS

J. J. Hassett

THE SOLID-SOLUTION INTERFACE

The adsorption or concentration of organic materials at the solid-solution interface is of particular importance in natural waters. Streams, lakes, and rivers contain a variety of colloidal materials both in their bottom sediments and dispersed throughout the aqueous phase. These colloids can actively sorb organic materials, removing them from solution or suspension, and hence can have a marked effect on the chemical and physiological properties of the organic pollutants.

The sediments in a natural body of water consist predominantly of organic colloids (such as clay minerals and metal oxides, hydroxides, and carbonates), of organic colloids, and of living organisms. The metal oxides and hydroxides and the organic colloids may exist as discrete particles or as coatings on other colloids such as the clay minerals. A major source of these inorganic colloids (and, to a certain extent, of the organic colloids) is the erosion of watershed soils. The properties of the sediments can be quite similar to those of the soils from which they are derived, or they may be substantially altered from the original soil, since the sediments may be subject to physical sorting by the water and often to different chemical environments (e.g., lower redox potentials).

Adsorption at the solid-liquid interface results when the forces of attraction between the surface (adsorbent) and the solute (adsorbate) overcome the forces of attraction between the solvent and the solute. Hence, the degree of adsorption depends on the relative strengths of the adsorbate-adsorbent interactions and the solute-solvent interactions. If the adsorbate-adsorbent interactions dominate due to a strong adsorbate-adsorbent interaction or due to a weak solvent-solute interaction, adsorption will take place and the adsorbing species will be primarily associated with the solid phase. The net interaction of the surface and the adsorbate may result from a variety of chemical and electrical interactions (Stumm and Morgan, 1970; Adamson, 1967).

ADSORPTIVE FORCES

1. *Coulombic attraction.* This force of attraction results when a charged surface such as a clay mineral attracts an oppositely charged ion to maintain electrical neutrality. The force of attraction is given by Coulomb's law:

$$F = q_1 q_2 / DX^2 \quad \text{(Eq. 1)}$$

where q_1 is the charge density of the surface, q_2 is the charge of the adsorbing species, D is the dielectric constant of the solvent and is a measure of the shielding of q_1 from q_2 by the solvent, and X is the distance between the charges. Sorption of inorganic cations by negatively charged soil colloids in the process of cation exchange is one example of coulombic attraction. The sorption of the organic cations paraquat and diquat by montmorillonite and kaolinite (Weber *et al.*, 1965) is also an example of coulombic attraction. In the case of paraquat and diquat sorption within the interlayer of montmorillonite, other sorptive forces add to the coulombic attraction.

2. *London-van der Waals dispersion forces* result from the oscillating electron cloud of one atom rotating in phase with a nonoverlapping oscillating electron cloud of another atom, producing a dipole-like attraction. The differential heats of adsorption are of the order of 1 to 2 kcal $mole^{-1}$ for small molecules and atoms. For large molecules the heats of adsorption may be much larger. Corkill *et al.* (1966) gave the heats of adsorption of methane, ethane, pentane and hexane on carbon black as being 3, 4.3, 9.2 and 11.4 kcal $mole^{-1}$.

3. *Orientation energy* results from the attraction of a permanent dipole for another permanent dipole. The resulting energy of attraction is less than 2 kcal $mole^{-1}$.

4. *Induction forces* result from the attraction of an induced dipole for the inducing species which can be either a permanent dipole or a charged site or species. This force often adds to the adsorptive forces present in cases of coulombic or orientation energy attraction. The energy of attraction is less than 2 kcal $mole^{-1}$.

5. *Hydrogen bonding* occurs in compounds such as water where electrons are unequally shared between the more electronegative oxygen and hydrogen. This arrangement results in a slight negative charge on the oxygen atom and a slight positive charge on the hydrogen atoms, producing (in the case of water) a dipole moment of 1.84 Debye units (Douglas and McDaniel, 1965). Hence, attraction is possible between dissimilarly charged sites of the adsorbate and the adsorbent. The energy of attraction ranges from 2 to 10 kcal $mole^{-1}$.

6. *Chemical forces* result when the adsorbate-adsorbent bond approaches an ordinary chemical bond in strength ($>>$10 kcal $mole^{-1}$). Chemical forces extend over only very short ranges and often result in the nature of the adsorbate being significantly different in the adsorbed state. Such adsorption is often termed chemisorption to distinguish it from the less specific low-energy physical sorption. It is often difficult to distinguish between chemical and physical sorption because a chemisorbed layer may have physically sorbed layers upon it.

For some solutes the attractive force of the adsorbate for the solid surface can play a subordinate role to the hydrophilic-hydrophobic balance of the solute with the solvent (Hance, 1967; Stumm and Morgan, 1970). This type of adsorption is of particular interest when considering the adsorption of organic molecules that are concentrated at the solid-solution interface because of the hydrophobic nature of their hydrocarbon parts. For this type of adsorption the effect of the adsorbent on the interfacial tension or surface free energy would appear to be an important consideration in explaining the observed phenomena. Conversely, some ions that show a strong affinity for the solvent (for example, ones that are highly hydrated) may stay in solution even if they are specifically attracted to the adsorbent.

Traube observed a regularity in the lowering of surface tension by members of three homologous series of esters, alcohols, and fatty acids (Kipling, 1965). The rule derived from that study states, in essence, that the tendency to adsorb organic compounds from aqueous solution increases with increasing molecular weight for members of a homologous series. Hence, adsorptive energy increases systematically for each additional CH_2 group.

Other general rules (Stumm and Morgan, 1970) concerning the adsorption of organics state that a polar adsorbent adsorbs the most polar constituent of a nonpolar solution in preference to the least polar constituent(s). In contrast, a nonpolar surface adsorbs the nonpolar component preferentially from a polar solution.

ADSORPTION ISOTHERMS

Several mathematical expressions--some with a theoretical basis and others entirely empirical in nature--have been employed to describe the relationship between the amount adsorbed and the equilibrium solution concentration. Those equations that have a theoretical basis can (if the assumptions each is based upon are met) provide valuable information about bonding or adsorption energies (affinities), adsorption maxima (capacities), and interfacial free energies. The empirical equations provide a framework for predicting the distribution of adsorbate between the solid and aqueous phases.

Langmuir Adsorption Isotherm

The Langmuir equation (1918), originally developed to describe the adsorption of a gas by a clean solid surface, has been used by numerous investigators to describe adsorption at the solid-liquid interface. The equation usually takes the following form (Veith and Sposito, 1977):

$$\frac{x}{m} = \frac{KbC}{(1 + KC)} \qquad \text{(Eq. 2)}$$

where
x/m = amount of adsorbate adsorbed per unit mass of adsorbent
C = the equilibrium concentration of the adsorbate in solution
K = a constant related to the bonding energy of the adsorbate to the adsorbent
b = adsorption maximum or capacity factor

Correct use of the equation requires that two assumptions be met:

1. That the adsorbed ions be bound in a monolayer on a homogeneous surface with localized sites.
2. That the energy of adsorption be the same for each molecule of adsorbate regardless of the degree to which the monolayer is completed.

Veith and Sposito (1977) have shown that it is necessary not only to meet the basic assumptions of the Langmuir equation but also to have an independent means of determining that the only process taking place is adsorption, since the Langmuir equation will also fit data obtained in situations where secondary precipitation is taking place. Other investigators (Stumm and Morgan, 1970; Kipling, 1965) have also cautioned that although a set of data may fit the equation, that fact is not of itself sufficient evidence that the assumptions have been met.

The normal application of the Langmuir equation to adsorption data involves a least-squares fitting of the data to a linear form of equation 2. At least three linear forms of the Langmuir equation have been used in adsorption studies:

$$C/(x/m) = 1/Kb=C/b \qquad \text{(Eq. 3)}$$

$$1/(x/m) = 1/b+1/KbC \qquad \text{(Eq. 4)}$$

$$(x/m) = b-(x/m)/KC \qquad \text{(Eq. 5)}$$

Equation 3 has been used extensively in adsorption studies involving soils. A plot of C/(x/m) against C for this equation should yield a straight line having a slope of 1/b and an intercept at 1/Kb. For equation 4 the plot would be 1/(x/m) against 1/C, yielding a slope of 1/Kb and an intercept at 1/b. This type of plot is very similar to the double-reciprocal or Lineweaver-Burk plot used in enzyme studies employing Michaelis-Menten kinetics. For equation 5 (x/m) is plotted against (x/m)/C, yielding a slope equal to 1/K and an intercept at b. This plot is of the same form as the Eadie-Hofstee plot (Hofstee, 1952; 1960) also employed in Michaelis-Menten kinetics.

Dowd and Riggs (1965) compared the statistical fit and the predictability of the three linear forms of the Michaelis-Menten equation, which have the same form as the Langmuir adsorption isotherm and its linear equations:

$$v = \frac{V_{max}C_s}{K + C_s} \qquad \text{(Eq. 6)}$$

$$C_s/v = K_m/V_{max}+C_s/V_{max} \qquad \text{(Eq. 7)}$$

$$1/v = 1/V_{max}+K_m/V_{max}C_s \qquad \text{(Eq. 8)}$$

$$v = V_{max}-K_m v/C_s \qquad \text{(Eq. 9)}$$

where

v = the initial velocity of the reaction

C_s = the concentration of the substrate

V_{max} = the maximum initial velocity

K_m = the Michaelis constant

They found that equation 7, which has the same form as equation 3, and equation 9, which has the same form as equation 5, gave comparable predictions of the two constants when the error in determining the dependent variable (i.e., v or x/m) was small, although equation 9 would better show deviations from linearity. Equation 9 gave the best results when the error associated with determining the dependent variable was large. These results are supported by Syers *et al.* (1973), who in a soil adsorption study compared the form of the Langmuir equation given in equation 3 with that of equation 5. Dowd and Riggs (1965) concluded that the Lineweaver-Burk or double reciprocal plot--equation 8, which has the same form as equation 4--should not be used even if it fits the data well.

Several nonlinear forms of the Langmuir equation are used in adsorption studies:

$$\theta = KC/(1+KC) \qquad \text{(Eq. 10)}$$

$$(x/m) = bC/(K'+C) \qquad \text{(Eq. 11)}$$

Equation 10 is the same as equation 2 except that adsorption is expressed in terms of the percentage of the monolayer that is occupied by adsorbate molecules. This results in b, the monolayer capacity, having a value of 1 unit of adsorption sites and disappearing from the adsorption equation. Equation 11 reduces to equation 2 if K' is replaced with $1/K$; hence, $K' = 1/K$.

Freundlich Adsorption Isotherm

To describe adsorption from dilute solutions, Freundlich (1922) applied the adsorption isotherm:

$$a = \alpha c^{1/n} \qquad \text{(Eq. 12)}$$

or in its more commonly used form:

$$(x/m) = KC^{1/n} \qquad \text{(Eq. 13)}$$

where

C = the equilibrium concentration in the solution after adsorption

a or x/m = the adsorption value

α, K, and 1/n = constants

In studies of the adsorption of a variety of organic compounds on charcoals Freundlich found the adsorption exponent 1/n to vary between 0.1 and 0.5.

The Freundlich adsorption equation is normally considered an empirical equation relating the amount adsorbed to the equilibrium adsorbate concentration. Kipling (1965) cites a derivation of the Freundlich equation by Henry (1922) based on combining an expression for the free energy of a surface with the Gibbs equation. The resulting equation defines the adsorption exponent in terms of the monolayer capacity and surface free energy:

$$(x/m) = KC^{(RT(x/m)m/(\sigma_0-\sigma_1))} \qquad \text{(Eq. 14)}$$

hence

$$1/n = (RT(x/m)m/(\sigma_0-\sigma_1) \qquad \text{(Eq. 15)}$$

where

$(x/m)m$ = the monolayer capacity

σ_0 = the surface free energy in contact with pure solvent

σ_1 = the surface free energy of the surface covered with a monolayer of solute

R = the gas constant

T = temperature

This equation is applicable to dilute solutions where Gibb's surface excess equals (x/m), the amount adsorbed.

When $1/n \simeq 1$ then the Freundlich isotherm reduces to a partition equation:

$$K = \frac{(x/m)}{C} = \frac{C_s}{C_w} \qquad \text{(Eq. 16)}$$

where

C_s = the concentration of adsorbate in the solid phase

C_w = the concentration of adsorbate in equilibrium with the adsorbed phase

Partition equations have been written for both adsorption and desorption (LaFleur, 1976):

$$K_f = \frac{C_s}{C_w} \text{ adsorption} \qquad \text{(Eq. 17)}$$

$$K_b = \frac{C_s}{C_w} \text{ desorption} \qquad \text{(Eq. 18)}$$

Usually $K_b > K_f$; that is, a given surface coverage will be in equilibrium with a greater concentration of the solute for an adsorption process than for the desorption process.

The Freundlich equation is normally statistically fit to adsorption data in its linear form:

$$\log(x/m) = \log K + 1/n \log C \qquad \text{(Eq. 19)}$$

A plot of log(x/m) against logC yields a slope of 1/n and an intercept equal to logK.

In many studies the difference in adsorption of an organic material by several soils has been correlated with the organic carbon content of the adsorbate. When the adsorption constants are put on an organic carbon basis, the differences in adsorption are often removed.

$$K_{OC} = \frac{K \times 100}{\%OC} \qquad \text{(Eq. 20)}$$

Gibbs Adsorption Equation

The Gibbs equation, originally derived for the adsorption at the liquid-liquid interface (Kipling, 1965) has been applied to the adsorption of solutes from dilute solutions by solid surfaces (Stumm and Morgan, 1970):

$$\Gamma_i = \frac{\partial\gamma}{\partial\mu_i} \qquad \text{(Eq. 21)}$$

$$\mu_i = \mu_i + RT\ln a_i \qquad \text{(Eq. 22)}$$

hence,

$$\Gamma_i = \frac{-1}{RT} \frac{\partial\gamma}{\gamma \ln a_i} \quad T,P.\ \text{all } \mu\text{'s except } \mu_i \text{ and } \mu_{H_2O} \text{ constant} \qquad \text{(Eq. 23)}$$

where

Γ_i = the adsorption density of component i

γ = the interfacial tension

μ_2 = the chemical potential

a_i = the activity of component i

The Gibbs equation defines adsorption in terms of the effect of a solute in either increasing or decreasing interfacial tension. The equation illustrates that solutes which lower the interfacial tension tend to be concentrated at the interface. Many organic substances tend to lower the interfacial tension and hence are accumulated at the interface.

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4 ANALYTICAL METHODS: SOIL THIN-LAYER CHROMATOGRAPHY

W. L. Banwart

The principle of thin-layer chromatography (TLC) and evidence of its widespread use are presented by Stahl (1965). The basis of all chromatographic separations is similar in that a mobile phase passes over a stationary phase and thereby transports different substances with varying speeds in the direction of the flow. Conventional TLC is a form of elution chromatography in which molecules of the test compounds are exchanged between the mobile and stationary phase as a solvent carrying the compounds migrates across a uniform thin layer of stationary phase fixed to a glass plate. The rate or relative rate of movement of the test compounds is dependent on their physical properties and on experimental parameters. The solvent employed may be water, an organic solvent, or a mixture of solvents allowing movement of the test compounds.

The mobility or migration distances of substances on the TLC chromatograms can be expressed in terms of their relative mobility, R_f (Stahl, 1965),

where $R_f = \dfrac{\text{distance of spot center from starting point}}{\text{distance of solvent from starting point.}}$

The use of relative mobilities provides reproducible data, whereas absolute mobilities, which are defined simply as the distances of the spot centers from the starting point, may vary considerably with experimental conditions.

Using TLC to study the mobility of compounds requires a method for documenting the substances' movement. The final position of the compounds on the chromatogram can be made visible with dye indicators, fluorescence under ultraviolet light (Pullan, Howard, and Perry, 1966), a bioassay (Helling, Kaufman, and Dieter, 1971), a spark-chamber apparatus (Pullan *et al*, 1966), a beta camera (Snyder, 1970), and autoradiography using X-ray film (Mangold, Kammereck, and Malins, 1962). In the last of these methods, chromatograms are developed using ^{14}C labeled test compounds; X-ray film is then exposed to the chromatogram for several days before development. The developed films make it possible to observe visually the movement of the test compounds and can be used for easy calculations of R_f values. For quantitative measurements, radioactive compounds on TLC plates can be counted directly by commercially available instruments such as strip scanners (Ravenhill and James, 1967) or by zonal analysis where small successive segments of the chromatogram are scraped from the plate and radio-assayed by liquid scintillation spectrometry (Brown and Johnston, 1962). Thin-layer chromatography has been used as a standard method for separating and identifying many synthetic and natural organic compounds (Maier and Mangold, 1964; Stahl and Mangold, 1975), including polynuclear aromatic hydrocarbons (Zoccolillo and Liberti, 1976; Candeli *et al*., 1975).

Soil thin-layer chromatography was introduced by Helling and Turner (1968). In soil TLC a uniform but relatively thin layer (often less than 1 mm) of a soil-water slurry is spread on TLC plates and allowed to dry. The soil then serves as the stationary phase interacting with compounds carried by the mobile phase. Soil TLC has provided a much simpler and faster way of determining compound mobilities in soil than the traditional leaching columns. Helling and Turner (1968) found that pesticide mobilities determined by soil TLC correlated well with published data. The mobility of substances on soil TLC plates have been reported by Helling and Turner (1968) as frontal R_f values where

$$R_f = \frac{\text{distance of frontal edge of spot or streak from starting point}}{\text{distance of solvent edge from starting point}}$$

Standard or reference compounds can be spotted on each plate to improve reproducibility.

Data obtained by soil TLC provide information of a nature somewhat different from that obtained with sorption isotherms or partition coefficients. A compound on a soil TLC chromatogram may move as a compact band or as a diffuse streak. From the type of movement it is possible to draw conclusions about the homogeneity of the soil material or of the compound itself. It is also possible to obtain a relative measure of the distance compounds might leach in a soil system when finite amounts of water are applied. R_b values have been used (Rhodes, Belasco, and Pease, 1970), where

$$R_b = \frac{\text{distance moved by bottom of spot}}{\text{distance traveled by solvent}}$$

to measure the relative soil depth through which essentially all of a given organic compound (pesticide) applied to a soil has leached. Thus, soil TLC provides some kinds of information that cannot be obtained strictly from adsorption constants or partition coefficients.

Data recalculated from Rhodes, Belasco, and Pease (1970) showed simple correlation coefficients of $r = 0.95$ between Freundlich K and frontal R_f values for four agricultural chemicals applied to two soils. Helling (1971c) reported highly significant negative correlation coefficients for soil adsorption of nonionic herbicides and R_f values of the same or chemically similar herbicides. As determined by leaching experiments, the mobilities of six organophosphorus insecticides (McCarty and King, 1966), three acidic herbicides (Hamaker, Goring and Youngson, 1966) and their five s-triazine herbicides (Harris, 1966) were inversely related to their adsorption by the soil. Data by Hance (1967), using two soils and 29 organic compounds, show correlation coefficients ranging from 0.85 to 0.91 for the amount of compound adsorbed by the soil and the R_f values for TLC using 40% aqueous ethanol as a solvent. Other workers (Martin and Synge, 1941; Stahl, 1965) have also discussed the relationship between K and R_f values. If a correlation between R_f (mobility) and K (adsorption isotherm) values for a given set of organic compounds can be established, it should be possible to predict K values for additional test compounds on a particular soil.

The greatest use of soil TLC to date has been the study of pesticide mobility in soils (Helling 1971a,b,c; Hance, 1967), but applying the technique to other mobile organic compounds should provide useful data.

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5 ANALYTICAL PROCEDURES: CHEMICAL ANALYSIS

J. C. Means

The analysis of trace organic compounds in water or bound to soil and sediment samples is a complicated task because of a number of factors. First, the water and soil or sediment may contain a wide variety of organic compounds of different polarities, molecular weights, and structures. Second, the affinities of different types of organic compounds for different soil-sediment types span a large range. Third, the solubilities of organic compounds in different solvents vary considerably. Fourth, interactions between soil components and many types of organic compounds are poorly understood.

In general, the process of analyzing trace organic components in water and soil or sediment samples may be divided into these tasks:

1. Quantitative recovery of the organic compound of interest
2. Separation of that compound from other types of organic compounds
3. Quantitation of the organic compound using spectroscopy, chromatography, and radioactivity or a combination of techniques.

RECOVERY OF ORGANIC COMPOUNDS FROM ENVIRONMENTAL SAMPLES

To accurately determine the amount of a given organic compound in a water sample or bound to a soil or sediment sample, the compound must be quantitatively recovered from the gross sample. In the case of a soil or sediment sample, recovery is routinely accomplished by extracting the compound from the soil in a Soxhlet apparatus. Depending upon the variety of compounds which require analysis, a single solvent, a series of solvents, or a mixture of solvents may be required. For example, a cyclohexane or benzene extraction (Sawicki, 1964; Hermann, 1974) is typically used to recover aliphatic and aromatic hydrocarbons from sediments, whereas a benzene and methanol mixture may be used to remove a broad spectrum of nonpolar and polar organics (Giger and Blumer, 1974; Blumer and Youngblood, 1976). Acetone has been used to extract polar organics and humic substances.* Regardless of the extraction procedure used, it is always necessary to perform recovery studies using a reference compound to verify that the expected extraction efficiencies are achieved.

Organic compounds may be quantatively recovered from water samples using one of three techniques. Compounds having low boiling points and low or intermediate polarities may be stripped from the water by passing a pure inert gas through the sample and collecting it in a trap containing a gas chromatographic column packing (e.g., Tenax GC) (Bellar and Lichtenberg, 1974; Kuo *et al.*, 1977). Soluble organic compounds may be recovered from water by a series of extractions using single or mixed solvents. In some analytical schemes, the pH of the water may be altered (i.e., made basic, neutral, and acidic) to achieve partial separation of compounds having ionizable functional groups. (U.S. EPA, 1977; Acheson *et al.*, 1976; Chang, 1976; Webb *et al.*, 1973). A third technique, one which has been used very successfully, is to collect organic compounds by sorption on purified activated carbon (Keith *et al.*, 1976) or on purified sorbant resins (e.g., XAD-2, 4, and 8) (Malcolm, Thurman, and Aiken, 1977; Junk *et al.*, 1974; Adams, Menzies, and Levins, 1977). These techniques have the advantage that the organics contained in a very large sample volume may be collected on a relatively small amount of resin. However, the recovery efficiencies for different types of organics adsorbed from the water and subsequently desorbed from the resin vary significantly. Therefore, the recovery of each compound of interest should be evaluated. Another advantage of the resin sorption technique is that both polar and nonpolar organics may be sorbed to the resin and eluted for analysis.

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*F. J. Stevenson, 1977: personal communication.

Once an extract has been prepared from either a solid or a water sample, it is usually necessary to reduce the volume so as to bring the concentrations of the extracted components into a detectable (ppm) analytical range. The best general technique available for this process is the use of a Kuderna-Danish evaporator (Webb *et al.*, 1973; U.S. EPA, 1977). In some cases air evaporation or evaporation under a stream of nitrogen may be sufficient, but several studies have shown that significant losses of extracted organics may occur (Chiba and Mosley, 1968; Goldberg, Delong, and Sinclair, 1973). Similarly, rotary vacuum evaporation may be appropriate for certain compounds, but losses of many extracted components may occur. Extracts are typically concentrated by a factor of 500 to 10,000, depending upon the origin of the extract and the sensitivity of the analytical systems being used. Here again, it is advisable to test the recovery efficiency for the compound of interest using the concentration technique being considered.

FRACTIONATION, CLEANUP, AND SEPARATION OF ORGANIC EXTRACT COMPONENTS

Organic extracts of soil or sediments and of water, particularly those from industrial areas, may contain hundreds of components. These multiple components tend to complicate the accurate quantitation of individual constituents. Therefore, some steps may be needed to fractionate the extract prior to analysis. To some extent, fractionation begins with the selection of an extracting solvent or sorption resin. However, solvent selectivities are rarely sufficient, especially when concentration factors are high. Solvent-solvent partitioning of the organics in an extract may be useful in crude fractionations (e.g., separating polar compounds from nonpolar compounds).

Liquid chromatography and thin-layer chromatography (TLC) provide the best selectivities in fractionating complex mixtures of organics. For relatively large extracts, separation on liquid chromatographic columns containing such adsorbents as silica gel, alumina, or Florisil is the method of choice. Excellent separations of complex mixtures from acidic, basic, and neutral fractions of coal wastes and cigarette-smoke condensates have been achieved using these three adsorbents (Swain, Cooper, and Stedman, 1969; Bell, Ireland, and Spears, 1969; Severson *et al.*, 1976).

In the last few years, a number of advances in liquid chromatographic column packings have provided investigators with a number of gel-permeation and adsorption materials which can be extremely useful in fractionating and separating complex mixtures into subsamples which can be analyzed and quantitated.

For relatively small samples, thin-layer chromatography can be used successfully to fractionate a complex mixture. The same basic substrates mentioned above for use in column chromatography are used for TLC separations. Careful selection of solvents and the use of two-dimensional development can yield excellent purifications of individual components prior to quantitation. A large number of investigators have employed TLC to purify compounds for study or to fractionate extracts prior to quantitative analysis (Treiber, 1976; Grant and Meiris, 1977; Bender, 1968; White and Howard, 1967; Pierce and Katz, 1975; Stanley, Bender, and Elbert, 1973; additional references are given in the analytical techniques section of the bibliography at the end of this report).

QUANTITATION OF TRACE ORGANIC COMPOUNDS IN SOLVENT EXTRACTS

The quantitation of individual components of a complex mixture after partial cleanup or fractionation may generally be achieved using the techniques of spectroscopy, gas chromatography, liquid chromatography, or, in appropriate cases, liquid scintillation counting or combinations of the above techniques.

Spectroscopic techniques, which are based on some characteristic absorption wavelength (in the UV, visible, or infrared spectrum) of the compound or a derivative, vary in their selectivity and sensitivity. In cases where the extracts contain relatively few components, spectroscopic methods may be successfully used to quantitate a component without additional cleanup or separation. In most cases, however, the spectroscopic techniques must be used in combination with compatible separation systems (e.g., liquid chromatography or thin-layer chromatography). A large body of literature exists on separations and quantitations of organic pollutants using the above techniques. Representative reports are those of Caton, Matthews, and Walters (1976); Kelly (1967); Willis (1973); Freudenthal *et al.* (1975); Jenkins and Baird (1975); Brocco, Cantuti, and Cartoni (1970); and IUPAC Applied Chemistry Division (1974). Additional references are listed in the bibliography.

One spectroscopic technique which offers a relatively high degree of both selectivity and sensitivity is the use of fluorescence spectra of various compounds or their fluorescent derivatives (Woo *et al.*, 1978). These techniques are particularly useful when combined with liquid chromatography for the analysis of many coal-derived substances (Stroupe *et al.*, 1977) and pesticides (Mallet, Belliveau, and Frei, 1975). All of these spectroscopic techniques have the advantage that they are not destructive to the sample being analyzed and that the column packing materials and thin-layer supports used for separations prior to spectral analysis can cover an almost unlimited range of molecular weights.

Gas chromatography (GC) is perhaps the most widely used technique for the separation and quantitation of organic compounds. Methods are available for almost every class of organic pollutant including many energy-related compounds. Column packing materials are available for the separation of compounds representing a broad spectrum of polarities and functional groups. Although fewer liquid phases are readily available, capillary columns have demonstrated increasing utility for the separation of the highly complex mixtures of organics typically found in environmental extracts.

Gas chromatographic separations in general are better than those offered by liquid chromatography, but the compounds which can be analyzed by GC are limited to those having significant vapor pressures at temperatures below 400°C. In most cases, gas chromatographic analysis is destructive of the sample. A wide variety of GC detector systems are available. The flame ionization detector is the most common universal type. A number of other types of detectors demonstrate selectivities for specific types of compounds (e.g., the electron capture detector for halogens, the thermionic detector for nitrogen and phosphorus, and the flame photometric detector for sulfur and phosphorus). All of these detection systems may be used to quantitate organic compounds with the use of appropriate internal standardization techniques. The literature contains a large amount of information on this general topic. Pertinent references are included in the bibliography.

In the last decade, gas chromatography has been combined with mass spectrometry, providing investigators with a very powerful analytical system which can be used to both identify and quantitate organic compounds (John and Nickless, 1977; Janini *et al.*, 1976; Alford, 1977; Oswald, Albro, and McKinney, 1974; O'Reilly and Murrmann, 1974; Lao, Thomas, and Monkman, 1975; and McGuire, Alford, and Carter, 1973).

In certain types of experiments, radiolabeled organic compounds may be used successfully to follow the movement of trace organics in environmental samples. When labeled compounds are used, many types of samples may be analyzed directly without the need for extraction, concentration, or cleanup procedures. Care must be taken, however, to insure that the labeled compound introduced into the experimental system is not degraded in such a way that the radioactivity is lost or transferred to other compounds. The sample is typically separated by (1) thin-layer chromatography followed by radioautography or liquid scintillation counting or (2) by liquid chromatography followed by liquid scintillation spectrometry. Carbon -14 or tritium -3 labeled compounds can be detected in liquid samples by liquid scintillation spectrometry on aliquots of the samples. If solid samples are to be analyzed, the radiolabeled compound may be extracted and then analyzed as a liquid sample. Solids may also be analyzed directly by pyrolytic combustion of the solid and recovery of the radioactivity as $^{14}CO_2$ or $^{3}H_2O$.

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6 REVIEW AND INTERPRETATION OF ADSORPTION DATA

K. A. Reinbold and J. J. Hassett

A review of the literature revealed relatively few data on the adsorption of energy-related organic pollutants by sediments or soils. The summary presented here, therefore, covers literature on a variety of types of organic compounds, including pesticide data from references not covered by Farmer (1976).

Some of the published reports included constants for the sorption of organic compounds on various adsorbents. These constants are tabulated at the end of this chapter. However, many sources containing sorption data did not report sorption constants. The latter publications are included in the bibliography.

Except in the case of pesticides, most of the adsorption constants reported for organics were derived using adsorbents other than sediments, soils, and clay minerals. The most commonly used adsorbents were activated carbon or ion exchange resins, which are often used for the removal of organics in water treatment processes. Nylon and cellulose triacetate have also been used. The pesticide data, however, do pertain to sorption on sediments, soils, or clay minerals. The adsorption constants were determined in most cases by fitting experimentally derived data to various forms of the Freundlich or Langmuir adsorption equations.

FACTORS INFLUENCING ADSORPTION

Adsorption is a process in which a solution component is concentrated at the solid-solution interface. Adsorption results when the forces of attraction between the solution component and the surface, that is, the adsorbate-adsorbent interaction, overcomes the forces of attraction between the solution component and the solvent, that is, the solute-solvent interaction. There are two general cases where the adsorbate-adsorbent interaction is greater than the solute-solvent interaction and adsorption results.

In the first case there is a strong positive interaction between the surface and the adsorbate, and this interaction is strong enough to overcome even a fairly strong solute-solvent interaction. In this case adsorption is primarily related to the nature of the bonding between the adsorbate and the adsorbent. The adsorption of organic cations such as paraquat by clay minerals or polar organic molecules within the montmorillonitic interlayer are examples of this type of adsorption (Weber *et al.*, 1965). Reviews emphasizing the effect of adsorbate and adsorbent properties on adsorption have been written by Mortland (1970), Adams(1973), Bailey and White (1970), and Weber (1972).

In the second case, adsorption takes place not because of a strong adsorbate-adsorbent interaction, but rather due to a weak solute-solvent interaction. In this case even a small positive adsorbate-adsorbent interaction can overcome the solute-solvent interaction and result in adsorption. The degree of adsorption or partitioning of the adsorbing material between the solid and aqueous phases is primarily determined by the suitability of the aqueous phase as a solvent for the material. The poorer the aqueous phase as a solvent for the adsorbing species, the weaker the solute-solvent interaction and the greater the adsorption.

The adsorption of nonpolar aromatic hydrocarbons of low water solubility by organic surfaces is an example of this type of adsorption (Karickhoff *et al.*, 1979; Means *et al.*, 1979). This type of adsorption has been called "hydrophobic adsorption" because of the emphasis on the weak solute-solvent interaction in determining the degree of adsorption in aqueous systems (Horvath and Melander, 1978)

Hydrophobic or nonpolar adsorption can be considered an example of a nonpolar organic compound (adsorbate) partitioning between a polar aqueous phase and a stationary organic phase (adsorbent). In a soil or sediment system the aqueous phase would be the soil solution or the interstitial water in the sediment, while the organic phase would be the naturally occurring humic materials. Factors which either increase the affinity of the adsorbate for the humic surfaces or decrease the affinity of the adsorbate (solute) for the solvent (water) would result in greater adsorption.

Van der Waals forces have been identified as the main source of adsorbate-adsorbent interactions between nonpolar compounds and nonpolar organic surfaces (Horvath and Melander, 1978). The differential heats of adsorption for van der Waals forces are of the order of 1 to 2 kcal mole^{-1} for small molecules; these forces may be much greater for larger molecules, especially with an increase in the number of double and triple bonds (Bailey and White, 1970). This is illustrated by the adsorption of methane, ethane, pentane and hexane by carbon black. These hydrocarbons gave differential heats of adsorption of 3, 4.3, 9.2 and 11.4 kcal mole^{-1}, respectively (Corkill *et al.*, 1966). The differential heats of adsorption do not increase indefinitely with increasing molecular size; eventually a point is reached where increasing molecular size does not increase adsorption and may even decrease adsorption due to steric hindrance.

Many factors influence the solute-solvent interaction and hence influence adsorption. Molecular properties such as chain length, molecular volume, molecular weight, carbon number, and polarity have all been shown to influence adsorption (Bailey and White, 1970; Gustafson and Paleos, 1971; Lailach *et al.*, 1968; Cummings *et al.*, 1959; Bartell and Miller, 1924; Kipling, 1965; Hansen and Craig, 1954; Parkash, 1974). It has been demonstrated that as chain length, molecular volume, molecular weight, and carbon number increase, and as polarity decreases, the solute-solvent interaction weakens and hydrophobic adsorption increases. The effect of all of these properties on the solute-solvent interaction is integrated into the water solubility of the compound.

The adsorption of hydrophobic compounds has been shown to increase with decreasing water solubility of the compound (Karickhoff *et al.*, 1979; Means *et al.*, 1979). The adsorption of more polar compounds has also been shown to increase with decreasing water solubility, but only within a family of compounds (Bailey and White, 1970). Aqueous solubilities of organic compounds, while useful in predicting adsorption, are often difficult to determine. Some of the difficulties encountered include the approach of the water solubilities to analytical detection limits, the formation of stable suspensions and the long equilibration times required to establish equilibrium.

Lambert (1968) discussed the similarity between the role of soil organic matter in the sorption of organic compounds and the role of an organic solvent in a liquid-liquid extraction. He observed that the partitioning of a nonpolar organic compound between the soil solution and soil organic matter was highly correlated with the partitioning of the compound between water and an organic solvent. Karickhoff *et al.* (1979) reported, for sorption placed on an organic carbon basis (Koc), a significant correlation between the sorption of several aromatic hydrocarbons and the partitioning of the compounds between octanol and water (Kow).

$$\log Koc = 1.00 \log Kow - 0.21 \qquad \text{(Eq. 24)}$$

The linear partition coefficients (Kp) for many compounds may be calculated from the following equation:

$$Kp = Cs/Cw \qquad \text{(Eq. 25)}$$

where

Cs = the concentration of the compound in the solid phase at equilibrium

Cw = equilibrium solution concentration of the compound

When the individual linear partition coefficients for the sorption of a hydrophobic organic compound by a variety of different sediments and soils are divided by the respective sediment or soil organic carbon contents, a unique constant Koc is produced.

$$Koc = \frac{Kp \times 100}{\%OC} \qquad \text{(Eq. 26)}$$

This constant is independent of soil or sediment (adsorbent) properties and is only dependent on the nature of the adsorbing species (Karickhoff *et al.*, 1979; Means *et al.*, 1979).

The relationship between Koc values and Kow values for hydrophobic compounds has several distinct merits. First, Kow determinations are more reliable than water solubility determinations, particularly for the highly hydrophobic compounds. Second, once a compound's Kow value has been measured or calculated, its Koc can be determined from equation 24. Third, if the organic carbon contents of the individual soils or sediments are known, then their respective Kp values for the adsorption of the compound can be calculated.

Table 5 gives an example of linear Kp values, measured Koc values and Koc values calculated from Kow values for the sorption of three hydrophobic compounds, pyrene, dibenzothiophene and acetophenone by a variety of sediments.

TABLE 5. Kow, CALCULATED Koc, LINEAR Kp AND MEASURED Koc VALUES FOR SORPTION OF PYRENE, DIBENZOTHIOPHENE AND ACETOPHENONE BY SOILS AND SEDIMENTS

Compound	Kow	Koc (calc'd)	Sample		Kp	Koc (meas'd)	Average Koc
			No.	%OC			
Pyrene	124,000	76,400	B2	1.21	774	63,991	63,400
			4	2.07	1098	53,019	
			5	2.28	1191	52,250	
			6	0.72	633	87,847	
			8	0.15	125	83,333	
			9	0.11	79	71,818	
			14	0.48	285	59,271	
			15	0.95	783	82,453	
			18	0.66	509	77,182	
			20	1.30	747	57,469	
			21	1.88	1159	61,628	
			22	1.67	811	48,557	
			23	2.38	1130	47,487	
			26	1.48	1023	69,108	
Dibenzothiophene	24,000	14,700	B2	1.21	117.5	9711	11,230
			4	2.07	180.6	8725	
			5	2.28	167.1	7329	
			6	0.72	60.8	8444	
			8	0.15	9.4	6267	
			9	0.11	5.8	5273	
			14	0.48	49.7	10,354	
			15	0.95	179.9	18,937	
			18	0.66	65.1	9864	
			20	1.30	101.4	7800	
			21	1.88	276.0	14,681	
			22	1.67	176.3	10,557	
			23	2.38	388.6	16,328	
			26	1.48	134.5	9088	
Acetophenone	38.6	23.8	B2	1.21	0.44	36	38.6
			4	2.07	0.89	43	
			5	2.28	0.56	24	
			6	0.72	0.68	95	
			8	0.15	0.07	48	
			9	0.11	0.09	82	
			14	0.48	0.12	25	
			15	0.95	0.27	28	
			18	0.66	0.30	46	
			20	1.30	0.29	22	
			21	1.88	0.85	45	
			22	1.67	0.53	31	
			23	2.38	0.68	29	
			26	1.48	0.66	45	

The range in Kp values for the adsorption of hydrophobic compounds depends on the compound being adsorbed and the range in organic carbon contents found in the soils or sediments studied. The upper limit for Koc values depends on the compound, but appears to be around 2,000,000 due to present analytical chemistry limitations. The lower limit for the validity of the Koc-Kow relationship has not yet been defined. This limit will be reached when case 1 adsorption, i.e., a specific strong adsorbate-adsorbent interaction, is encountered.

A relationship has been demonstrated for nonlinear Freundlich isotherms when the data are expressed on a molar basis instead of a mass basis (Osgerby, 1970). Molar Kd values may be calculated from mass Kd values by the following equation:

$$\mathrm{Kd(Molar)} = \frac{\mathrm{Kd(Mass)} \times \mathrm{Molecular\ weight}^{1/n}}{\mathrm{Molecular\ weight}} \qquad \text{(Eq. 27)}$$

Where Kd(Mass) and 1/n are Freundlich constants and the molecular weight is that of the adsorbate.

INTERPRETATION OF TABULATED DATA

Various combinations of the influencing factors discussed above are necessary to explain the adsorption data obtained from the literature and tabulated at the end of this chapter. For the nonpesticide organics, the adsorbents used in most of the studies reviewed were montmorillonite clay or carbon rather than natural sediments or soils. Thus, rather than a variety of adsorbents with a range of characteristics, two distinctly different types are represented: an inorganic clay mineral and an organic.

The chemical characteristics of the adsorbate account for much of the variation in adsorption behavior shown in the tabulated data. These effects were best shown in studies of groups of related compounds. Linner and Gortner (1935) studied the adsorption of 31 organic acids on carbon; the results are summarized in Table 6. Traube's rule that adsorption from aqueous solutions increases with molecular weight for a homologous series was demonstrated for fatty acids but not for other acids. The branched chain had little effect on the maximum adsorption of the acids, but the double bond showed a tendency to decrease adsorption. The introduction of polar groups--carboxyl, hydroxyl, or keto--caused decreased adsorption. The decrease was more pronounced as the number of carboxyl groups increased or as a second hydroxyl group was introduced. The decrease in adsorption caused by the keto group was dependent on the length of the chain and the position of the polar group in the chain.

For 52 structurally related N-phenylcarbamates, acetanilides, and anilines from aqueous 2% ethanol solutions, the inverse relationship between solubility and adsorption accounted for 60 percent of the total variation in adsorption, shown by the data in Table 6 (Ward and Upchurch, 1965). All of the compounds were adsorbed on nylon and cellulose triacetate. Other than solubility, the principal variable factor affecting adsorption was the difference in the molecular structures of the compounds. An investigation of compounds having systematic variations in molecular structure shows which sites in the molecule can be involved in adsorptive processes and how various substituents may influence the extent of adsorption. For those compounds, differences in molecular structure caused differences in adsorption as a result of steric hindrance, tautomerism, chelation, and induction. The results suggest that the preferred adsorption mechanism of the amido compounds from aqueous solution is via the adsorbate's imino hydrogen and the adsorbent's carbonyl oxygen. If neither of these is available, however, alternative binding sites are utilized.

As a means of establishing a quantitative relationship between soil sorption equilibria and chemical structure, Lambert (1967) proposed the following relationship between parachor of uncharged organic chemicals for which no appreciable hydrogen bonding occurs and the soil sorption of those chemicals:

$$K_e = aP\hat{\Delta}U \qquad \text{(Eq. 25)}$$

The relationship is based upon extrathermodynamic linear free energy approximations and uses of parachor as an approximate measure of the molar volume of the chemical. Distribution equilibria between soil and water for a number of chemical homologs of two chemical classes, including anilines (see Table 6) were used to establish the relationship. The relationship emphasizes the importance of using the partition or distribution coefficient, defined with respect to organic matter, as the most representative index of soil sorption equilibria.

Hance (1969) extended this relationship. A factor given by (parachor-45N), where N is the number of sites in a molecule which can participate in the formation of a hydrogen bond, was correlated with the logarithm of the Freundlich K value for the adsorption of 29 aromatic herbicides. Again, the relationship is valid for soils in which organic matter is the dominant adsorbing constituent.

In the case of a few compounds, adsorption constants were determined for more than one adsorbent (Table 6). Where data were obtained on both a clay mineral and a sediment, the adsorption was generally greater on the sediment. Some data on sediments and soils, including those for benz(a)pyrene, pyrene, methoxychlor, and carbaryl, show a correlation between adsorption and organic matter content (Table 6) (Smith, Mabey, Bohonos, Holt, Lee, Chou, Mill, and Bomberger, 1976a; Karickhoff, Brown, and Scott, 1978; La Fleur, 1976a).

In addition to the adsorption constants for specific compounds and adsorbents, additional pertinent data are tabulated here. Adsorption constants for a number of pesticides averaged over several soils are shown in Table 7. Also, Tables 8 and 9 show the inverse relationship between R_f values obtained by soil thin-layer chromatographs and adsorption or adsorbate characteristics.

(Note: the references cited in this chapter are listed beginning on p. 110.)

TABLE 6: ADSORPTION CONSTANTS FOR ORGANIC COMPOUNDS

Compound Name			Ref.

COMPOUNDS OTHER THAN PESTICIDES

Acids, Aliphatic

acetic acid

$C_2H_4O_2$

Compound properties[a]

m.w. 60.05

m.p. 16.604°C

b.p. 117.9°C

density 1.0492^{20}_{4}

water sol ∞

Adsorbent

nordite (decolorizing carbon)

Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$

$\alpha\beta$	α	β
0.462	0.266	1.736

Adsorption equation: $a = \alpha C^{1/n}$

α	$1/n$
2.46	0.351

Ref.: Linner and Gortner, 1935

Experimental Conditions: 1 gm of adsorbent and concentrations or reagents varying from 0.01 to 0.25 molar.

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[a] See notes at end of table

TABLE 6: *Continued*

Compound Name | **Ref.**

adipic acid

$C_6H_{10}O_4$

Compound properties

m.w. 146.14[a]

m.p. 151°C[a]

b.p. 265°C at 100mm[a]

density 1.360_4^{25}[a]

water sol 1.5^{15}[b]

Adsorbent

nordite (decolorizing carbon)

Adsorption equation: $a=\frac{\alpha\beta C}{1+\alpha C}$

αβ	α	β
2.347	1.886	1.245

Adsorption equation: $a=\alpha C^{1/n}$

α	1/n
1.79	0.163

Experimental Conditions: same as for acetic acid.

Ref.: Linner and Gortner, 1935

butyric acid

$C_4H_8O_2$

Compound properties[a]

m.w. 88.12°C

m.p. -4.26°C

b.p. 163.53°C

density 0.9577_4^{20}

water sol ∞

Adsorbent

nordite (decolorizing carbon)

Adsorption equation: $a=\frac{\alpha\beta C}{1+\alpha C}$

αβ	α	β
1.689	0.863	1.957

Adsorption equation: $a=\alpha C^{1/n}$

α	1/n
2.46	0.177

Experimental Conditions: same as for acetic acid.

Ref.: Linner and Gortner, 1935

TABLE 6: *Continued*

Compound Name			Ref.
butyric acid $C_4H_8O_2$ Compound properties[a] m.w. 88.12 m.p. -4.26 °C b.p. 163.53 °C density 0.9577^{20}_{4} water sol ∞	Adsorbent activitated charcoal B10	Adsorption equation: $y = a.x^b$ x - range I (mmol/dm^3) a b 0.08 - 7.18 0.878 0.4	Spahn et al., 1974
n-butyric acid	Adsorbent XAD-2 (amberlite resin)	Adsorption equation: $\frac{c}{q} = \frac{1}{Kb} + \frac{c}{b}$ (Langmuir) K(25°C) b(25°C) 23.7 liter/mole $1.46X10^{-3}$ mole/g Enthalpy of adsorption: $\Delta H° = 2.303 \frac{RT_1T_2}{(T_2-T_1)} (\log K_2' - \log K_1')$ q $-\Delta H°$* $7X10^{-4} \frac{mole}{q}$ 4.1 kcal/mole $9X10^{-4} \frac{mole}{q}$ 2.4 kcal/mole $1.2X10^{-3} \frac{mole}{q}$ 2.1 kcal/mole	Gustafson et al., 1968

*ΔH decreases with increasing surface coverage, i.e. energetically preferred sites are utilized first.

TABLE 6: *Continued*

Compound Name	Adsorbent	Adsorption equation	Ref.
caproic acid $CH_3(CH_2)_4CO_2H$ Compound properties m.w. 116.16^a m.p. −2 to $-1.5°C^a$ b.p. $205°C^a$ density $0.9274_4^{20\,a}$ water sol 0.4 gm/100 ml^b	nordite (decolorizing carbon)	Adsorption equation: $a= \frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ 8.772, α 4.636, β 1.892 Adsorption equation: $a= \alpha C^{1/n}$ α 3.03, $1/n$ 0.175	Linner and Gortner, 1935

Experimental Conditions: same as for acetic acid.

Compound Name	Adsorbent	Adsorption equation	Ref.
citraconic acid $C_5H_6O_4$ Compound properties m.w. 130.10^a m.p. $91°C^b$ density 1.617^a water sol 238 $cold^b$	nordite (decolorizing carbon)	Adsorption equation: $a= \frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ 1.356, α 1.014, β 1.337 Adsorption equation: $a= \alpha C^{1/n}$ α 1.69, $1/n$ 0.167	Linner and Gortner, 1935

Experimental Conditions: same as for acetic acid.

TABLE 6: *Continued*

Compound Name — Ref.

citric acid

$C_6H_8O_7$

Compound properties

m.w. 192.14[a]

m.p. 153°C (anhydrous)[a]

b.p. decomp[a]

density 1.542^{18}_{4}[b]

water sol 133 cold gm/100 ml[b]

Adsorbent

nordite (decolorizing carbon)

Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$

$\alpha\beta$	α	β
1.444	2.757	0.524

Adsorption equation: $a = \alpha C^{1/n}$

α	1/n
0.73	0.203

Ref.: Linner and Gortner, 1935

Experimental Conditions: same as for acetic acid.

dibromosuccinic acid

$C_4H_4O_2Br_2$

Compound properties[b]

m.w. 275.90

m.p. 151-3°C

Adsorbent

nordite (decolorizing carbon)

Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$

$\alpha\beta$	α	β
1.397	1.119	1.248

Adsorption equation: $a = \alpha C^{1/n}$

α	1/n
2.58	0.320

Ref.: Linner and Gortner, 1935

Experimental Conditions: same as for acetic acid.

TABLE 6: *Continued*

Compound Name			Ref.
formic acid HCO_2H Compound properties[a] m.w. 46.03 m.p. 8.4°C b.p. 100.7°C density 1.220_4^{20} water sol ∞	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ 0.273; α 0.159; β 1.710 Adsorption equation: $a = \alpha C^{1/n}$ α 2.47; 1/n 0.435	Linner and Gortner, 1935

$\alpha\beta$	α	β
0.273	0.159	1.710

α	1/n
2.47	0.435

Experimental Conditions: same as for acetic acid.

Compound Name			Ref.
fumaric acid $C_4H_4O_4$ Compound properties m.w. 116.07[b] m.p. 287°C[b] b.p. 200 subl.[b] 165 subl.[a] density 1.635_4^{20}[b] water sol 0.70^{25}; 9.8^{100}[b]	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ 7.097; α 5.798; β 1.224 Adsorption equation: $a = \alpha C^{1/n}$ α 2.81; 1/n 0.248	Linner and Gortner, 1935

$\alpha\beta$	α	β
7.097	5.798	1.224

α	1/n
2.81	0.248

Experimental Conditions: same as for acetic acid.

TABLE 6: *Continued*

Compound Name			Ref.
glutaric acid $C_5H_8O_4$ Compound properties m.w. 132.11^a m.p. $99°C^a$ b.p. 304 decomp.^{b} density $1.424^{25}_{4}{}^a$ water sol $64^{20}{}^a$	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$	Linner and Gortner, 1935

$\alpha\beta$	α	β
3.697	3.104	1.192

Adsorption equation: $a = \alpha C^{1/n}$

α	1/n
1.96	0.201

Experimental Conditions: same as for acetic acid.

glyceric acid $C_3H_6O_4$ Compound properties^a m.w. 106.08 b.p. disintegrates water sol ∞	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$	Linner and Gortner, 1935

$\alpha\beta$	α	β
0.668	0.812	0.823

Adsorption equation: $a = \alpha C^{1/n}$

α	1/n
1.29	0.267

Experimental Conditions: same as for acetic acid.

TABLE 6: *Continued*

Compound Name			Ref.
glycolic acid $HOCH_2CO_2H$ Compound properties[a] m.w. 76.05 m.p. 80°C b.p. decomposes	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ 0.239, α 0.249, β 0.958 Adsorption equation: $a = \alpha C^{1/n}$ α 1.54, $1/n$ 0.390	Linner and Gortner, 1935
glyoxylic acid $C_2H_2O_3$ Compound properties m.w. 74.04[a] m.p. 70-5°C[a] (+1/2w) 98 (anhydrous) water sol very soluble[b]	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ 0.508, α 0.223, β 2.275 Adsorption equation: $a = \alpha C^{1/n}$ α 3.89, $1/n$ 0.455	Linner and Gortner, 1935

glycolic acid — Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$

$\alpha\beta$	α	β
0.239	0.249	0.958

Adsorption equation: $a = \alpha C^{1/n}$

α	$1/n$
1.54	0.390

Experimental Conditions: same as for acetic acid.

glyoxylic acid — Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$

$\alpha\beta$	α	β
0.508	0.223	2.275

Adsorption equation: $a = \alpha C^{1/n}$

α	$1/n$
3.89	0.455

Experimental Conditions: same as for acetic acid.

TABLE 6: *Continued*

Compound Name			Ref.
isobutyric acid $(CH_3)_2CHCO_2H$ Compound properties m.w. 88.11^a m.p. $-46.1°C^a$ b.p. $153.7°C^a$ density 0.96815_4^{20a}; $.949_4^{20b}$ water sol 20 ^{20} gm/100 ml^b	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a= \frac{\alpha\beta C}{1+\alpha C}$	Linner and Gortner, 1935

$\alpha\beta$	α	β
0.883	0.497	1.776

Adsorption equation: $a= \alpha C^{1/n}$

α	1/n
2.36	0.273

Experimental Conditions: same as for acetic acid.

Compound Name			Ref.
isovaleric acid $C_5H_{10}O_2$ Compound properties m.w. 102.13^a m.p. $-29.3°C^a$ b.p. $176.7°C^a$ density 0.9286_4^{20a} water sol 4.2^{20b}	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a= \frac{\alpha\beta C}{1+\alpha C}$	Linner and Gortner, 1935

$\alpha\beta$	α	β
1.630	0.902	1.807

Adsorption equation: $a= \alpha C^{1/n}$

α	1/n
2.51	0.227

Experimental Conditions: same as for acetic acid.

TABLE 6: *Continued*

Compound Name			Ref.
itaconic acid $C_5H_6O_4$ Compound properties m.w. 130.10[a] m.p. 175°C[a] b.p. decomposes[a] density 1.632[b] water sol 8.33^{20}[b]	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a= \frac{\alpha\beta C}{1+\alpha C}$ αβ α β 1.167 0.904 1.291 Adsorption equation: $a= \alpha C^{1/n}$ α 1/n 1.54 0.148	Linner and Gortner, 1935
	Experimental Conditions: same as for acetic acid.		
lactic acid (DL) $C_3H_6O_3$ Compound properties m.w. 90.08[a] m.p. 18°C[a] b.p. 122°C[a] density 1.249^{15}[b] water sol ∞[b]	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a= \frac{\alpha\beta C}{1+\alpha C}$ αβ α β 0.437 0.415 1.054 Adsorption equation: $a= \alpha C^{1/n}$ α 1/n 1.66 0.335	Linner and Gortner, 1935
	Experimental Conditions: same as for acetic acid.		

TABLE 6: *Continued*

Compound Name			Ref
levulinic acid $C_5H_8O_3$ Compound properties m.w. 116.13[a] m.p. 37.2 °C[a] b.p. 246°C slight decomp.[a] density 1.1335^{20}_{4}[a]; 1.1395^{20}_{4}[b] water sol very sol[b]	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a=\frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ α β 2.990 2.289 1.307 Adsorption equation: $a=\alpha C^{1/n}$ α $1/n$ 1.83 0.183	Linner and Gortner, 1935
	Experimental conditions: same as for acetic acid		
maleic acid $C_4H_4O_4$ Compound properties m.w. 116.07[a] m.p. 139-140°C[a] b.p. 135 decomp.[b] density 1.590^{20}_{4}[ba] water sol 78.8^{25}; $392.6^{97.5}$[b]	Adsorbent nordite (decolorizing (carbon)	Adsorption equation: $a=\frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ α β 1.233 0.884 1.395 Adsorption equation: $a=\alpha C^{1/n}$ α $1/n$ 1.90 0.203	Linner and Gortner, 1935
	Experimental conditions: same as for acetic acid		

TABLE 6: *Continued*

Compound Name			Ref
malic acid (l) $C_4H_6O_5$ Compound properties^{b} m.w. 134.09 m.p. 100°C b.p. 140°C decomp. density 1.595 water sol very sol	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ α β 0.531 0.574 0.927 Adsorption equation: $a=\alpha C^{1/n}$ α 1/n 1.28 0.252	Linner and Gortner, 1935
	Experimental conditions: same as for acetic acid		
malonic acid $C_3H_4O_4$ Compound properties m.w. 104.06^{b} m.p. 135.6°C subl.^{b} b.p. decomp. at 140°C^{a} density 1.631$_{4}^{15b}$; 1.619^{a} water sol 61.1^{0} gm/100 ml^{b} 73.5^{20} gm/100 ml^{b} 92.6^{50} gm/100 ml^{b}	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ α β 1.897 1.540 1.232 Adsorption equation: $a=\alpha C^{1/n}$ α 1/n 3.88 0.410	Linner and Gortner, 1935
	Experimental conditions: same as for acetic acid		

TABLE 6: *Continued*

Compound Name			Ref
mesaconic acid $C_5H_6O_4$ Compound properties m.w. 130.10^a m.p. 204.5 b.p. 250°C decomp.^{b} density 1.466_4^{20}g/ml^b water sol 2.7^{18b}; 118^{100b}	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a=\frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ 2.706, α 1.886, β 1.435 Adsorption equation: $a=\alpha C^{1/n}$ α 1.80, $1/n$ 0.133	Linner and Gortner, 1935
	Experimental conditions: same as for acetic acid		
methylsuccinic acid $C_5H_8O_4$ Compound properties^b m.w. 132.11 m.p. 111°C b.p. decomp. density 1.410g/ml water sol 66.7^{20}	Adsorbent nordite (decolorizing carbon)	Adsorption equation: $a=\frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ 0.664, α 0.608, β 1.092 Adsorption equation: $a=\alpha C^{1/n}$ α 1.30, $1/n$ 0.172	Linner and Gortner, 1935
	Experimental conditions: same as for acetic acid		

TABLE 6: *Continued*

Compound Name	Adsorbent	Adsorption equation	Ref
monobromosuccinic acid $C_4H_5O_4Br$ Compound properties m.w. 197.00^b m.p. 159°C^b 161°C^a density 2.073^a water sol 19^{15b}	nordite (decolorizing carbon)	Adsorption equation: $a=\frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ / α / β 0.934 / 0.643 / 1.451 Adsorption equation: $a=\alpha C^{1/n}$ α / 1/n 1.82 / 0.195	Linner and Gortner, 1935
Experimental conditions: same as for acetic acid			
oxalic acid $C_2H_2O_4$ Compound properties m.w. 90.04^a m.p. 189.5°C^a b.p. 157°C subl.^{a} density 1.900$_4^{17a}$ water sol 19.5^{15} gm/100ml^b 120^{90} gm/100ml^b (hydrated form)	nordite (decolorizing carbon)	Adsorption equation: $a=\frac{\alpha\beta C}{1+\alpha C}$ $\alpha\beta$ / α / β 0.440 / 0.332 / 1.325 Adsorption equation: $a=\alpha C^{1/n}$ α / 1/n 3.62 / 0.551	Linner and Gortner, 1935
Experimental conditions: same as for acetic acid			

TABLE 6: *Continued*

<table>
<tr><th>Compound Name</th><th></th><th></th><th>Ref.</th></tr>
<tr>
<td>propionic acid
$C_3H_6O_2$
Compound properties[a]
m.w. 74.08
m.p. -20.8°C
b.p. 140.99°C
density 0.9930^{20}
water sol =</td>
<td>Adsorbent
nordite (decolorizing carbon)</td>
<td>Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$
<table><tr><th>αβ</th><th>α</th><th>β</th></tr><tr><td>0.925</td><td>0.491</td><td>1.885</td></tr></table>
Adsorption equation: $a = \alpha C^{1/n}$
<table><tr><th>α</th><th>1/n</th></tr><tr><td>2.46</td><td>0.236</td></tr></table></td>
<td>Linner and Gortner, 1935</td>
</tr>
<tr><td></td><td colspan="2">Experimental conditions: same as for acetic acid.</td><td></td></tr>
<tr>
<td>propionic acid
$C_3H_6O_2$
Compound properties
m.w. 74.08
m.p. -20.8°C
b.p. 140.99°C
density 0.9930^{20}
water sol =</td>
<td>Adsorbents
Activated charcoal B10</td>
<td>Adsorption equation: $y = a \cdot x^b$
Adsorption constants:
<table><tr><th>x-range I (mmol/dm^3)</th><th>a</th><th>b</th></tr><tr><td>0.1 - 8.3</td><td>0.497</td><td>0.4</td></tr></table></td>
<td>Spahn et al., 1974</td>
</tr>
</table>

TABLE 6: *Continued*

Compound Name	Adsorbent	Adsorption equation	Ref.
pyruvic acid $C_3H_4O_3$ Compound properties m.w. 88.06[a] m.p. 13.6°C[a] b.p. 165°C slight decomp.[b] density 1.2272^{20}_{4}[a] water sol ∞[b]	nordite (decolorizing carbon)	Adsorption equation: $a= \frac{\alpha\beta C}{1+\alpha C}$ αβ: 0.979; α: 0.585; β: 1.674 Adsorption equation: $a= \alpha C^{1/n}$ α: 2.44; 1/n: 0.273	Linner and Gortner, 1935
Experimental Conditions: same as for acetic acid.			
succinic acid $C_4H_6O_4$ Compound properties[b] m.w. 118.09 m.p. 185°C b.p. 235°C dissint. density 1.564^{15}_{4} g/ml water sol 6.8 at 20°C 121 at 100°C	nordite (decolorizing carbon)	Adsorption equation: $a= \frac{\alpha\beta C}{1+\alpha C}$ αβ: 0.865; α: 0.467; β: 1.854 Adsorption equation: $a= \alpha C^{1/n}$ α: 2.44; 1/n: 0.273	Linner and Gortner, 1935
Experimental Conditions: same as for acetic acid.			

TABLE 6: *Continued*

Compound Name			Ref
tartaric acid			

$C_4H_6O_6$

Compound properties

m.w. 150.09^b

m.p. $100°C^b$

density 1.697^b; 1.788^a

water sol 20.6^{20b}; 9.23^{0b}; 185^{100b}

Adsorbent

nordite
(decolorizing
carbon)

Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$

$\alpha\beta$	α	β
0.322	0.468	0.687

Adsorption equation: $a = \alpha C^{1/n}$

α	$1/n$
0.94	0.275

Ref: Linner and Gortner, 1935

Experimental conditions: same as for acetic acid

valeric acid

$CH_3(CH_2)_3CO_2H$

Compound properties

m.w. 102.13^a

m.p. $-33.83°C^a$

b.p. $186.05°C^a$

density 0.9391_4^{20a}; 0.942_4^{20b}

water sol 3.7gm/$100ml^b$

Adsorbent

nordite
(decolorizing
carbon)

Adsorption equation: $a = \alpha C^{1/n}$

α	$1/n$
2.84	0.182

Adsorption equation: $a = \frac{\alpha\beta C}{1+\alpha C}$

$\alpha\beta$	α	β
1.878	0.872	2.154

Ref: Linner and Gortner 1935

Experimental conditions: same as for acetic acid

TABLE 6: *Continued*

Compound Name		Ref
Acids, Aromatic		
benzoic acid $C_7H_6O_2$ Compound properties m.w. 122.13[a] m.p. 122.4°C[a] b.p. 249°C[b] density 1.2659^{15}_{4} [b] water sol 0.18^{4} [b] 0.27^{18} [b] 2.2^{75} [b]	Adsorbents Type BL - activated carbon (Pittsburgh Chemical Co.) Surface area 1000-1100 μ^2/g Adsorption equation: $\frac{x}{m} = \frac{abC}{(1+aC)}$ Adsorption constants:	Ward and Getzen, 1970

Compound	pka	pH of soln.	a*	b	x/m
benzoic acid	4.20	3	0.238	510	489
		7	0.108	124	113
		11	0.081	75	67
-2,4-dichloro	2.76	3	0.259	676	651
		7	0.123	159	147
		11	0.108	73	69
-3-amino-2,5-dichloro (amiben)	3.40	3	0.928	515	510
		7	0.283	131	127
		11	0.025	72	51
-3-nitro-2,5-dichloro	3.23	3	0.360	505	491
		7	0.118	130	120
		11	0.035	93	72
-2-methoxy-3,6-dichloro (dicamba)	1.94	3	0.181	394	313
		7	0.317	154	149
		11	0.068	68	59

Experimental conditions: 100 ml aqueous acid solution: 10mg carbon

*Units: a = liters/μ mole
b = μ moles/g
c = μ moles/liter
$\frac{x}{m}$ = μ moles/g

TABLE 6: *Continued*

Compound Name			Ref.
benzoic acid $C_7H_6O_2$ Compound properties m.w. 122.13[a] m.p. 122.4°C[a] b.p. 249°C[b] density 1.2659_4^{15}[b] water sol 0.18^4[b] 0.27^{18} 2.2^{75}	Adsorbent activated charcoal B10	Adsorption equation: $y = a \cdot x^b$ Adsorption constant:	Spahn et al., 1974
benzoic acid and substituted benzoic acids $C_7H_6O_2$	Adsorbent charcoal, activated, 200 mesh	Adsorption equation: log x/m = log k + 1/n log c	Hartman, Kern, Bobalek, 1946

Spahn et al., 1974 — Adsorption constant:

x-range I (mmol/dm^3	a	b
0.1 - 6	3.06	0.181

Hartman, Kern, Bobalek, 1946:

1/n and log k Values

Acids	1/n	log k 20°	30°	40°	50°
Benzoic	0.3680	0.0613	0.0265	-0.1091	-0.2551
o-Chlorobenzoic	0.4060	0.2208	0.1834	0.1303	0.0936
o-Aminobenzoic	0.3693	0.3472	0.3031	0.2678	0.2218
o-Hydroxybenzoic	0.3840	0.2700	0.2385	0.2091	0.1844
o-Toluic	0.3879	-0.0215	-0.0719	-0.2510	-0.5232
m-Toluic	0.3581	-0.0092	-0.0582	-0.1791	-0.3732
p-Toluic	0.3696	0.1351	0.0762	-0.0324	-0.1886

Adsorption from benzene solutions.

TABLE 6: *Continued*

Compound Name	Adsorbent							Ref.
phenyl acetic acid								
$C_6H_5CH_2CO_2H$	Adsorbent Activated charcoal	Adsorption equation: $y = a \cdot x^b$						Spahn et al., 1974
Compound properties[a]								
m.w. 136.16								
m.p. 77°C		Adsorption constants:						
b.p. 265.5°C								
density 1.091^{77}_{4}; 1.228^{4}		x-range I (mmol/dm^3)	a	b	x-range II (mmol/dm^3)	a	b	
water sol slightly sol.	B10	0.1 - 10	2.51	0.16	0.001 - 0.1	2.6	0.32	
	LW	0.05 - 12	1	0.165				
	Lev 634	0.1 - 8	0.84	0.38	0.01 - 0.11	1.76	0.56	
	BD	0.1 - 22	1.14	0.15				
	D1	0.05 - 7	1.93	0.162				
	D2	0.1 - 8	1.57	0.245				
	B2	0.1 - 11	1	0.145				
	LS-supra	0.1 - 7	1.75	0.18	0.001 - 0.11	1.53	0.23	
	Decaka 9	0.1 - 8	1.82	0.03				
	106/427/1	0.1 - 7	1.53	0.11	0.001 - 0.12	2.05	0.33	
	106/427/5	0.1 - 6.5	1.87	0.144	0.001 - 0.11	1.85	0.3	
	106/427/3	0.1 - 8	2.08	0.244	0.001 - 0.12	2.6	0.44	

TABLE 6: *Continued*

Compound Name			Ref.
Carboxylic acids, aromatic Phenoxyacetic acid $C_8H_8O_3$ Compound properties m.w. 152.14 m.p. 99°C b.p. 285°C slight decomp. water sol 1.2¹⁰	Adsorbents Type BL - activated carbon (Pittsburgh Chemical Co.) Surface Area 1000-1100 μ^2/g	Adsorption equation: $\frac{x}{m} = \frac{abC}{(1+aC)}$ Adsorption constants:	Ward and Getzen, 1970

Adsorption constants:

Compound	pka	pH of soln.	a*	b	$\frac{x}{m}$
Phenoxyacetic Acid	3.03	3	0.423	446	436
		7	0.229	105	86
		11	0.209	64	43
-4-chloro-	2.36	3	0.362	575	560
		7	0.101	198	180
		11	0.115	145	133
-2,4-dichloro-	3.31	3	0.279	629	607
		7	0.112	223	205
		11	0.070	154	135
-2,4,6-trichloro-	3.35	3	0.672	676	666
		7	0.095	239	216
		11	0.073	144	127
2,4-dichloro-	3.92	3	0.431	645	630
		7	0.125	235	218
		11	0.100	59	54

Experimental Conditions: 100 ml aqueous acid solution: 10 mg carbon.

Units:
a = liters/μ mole
b = μ moles/g
c = μ moles/liter
$\frac{x}{m}$ = μ moles/g

TABLE 6: *Continued*

Compound Name			Ref.
2,4-dichloro-phenylacetic acid	**Adsorbents** Type BL - activated carbon (Pittsburgh Chemical Co.) Surface area 1000-1100 μ^2/g	Adsorption equation: $\frac{x}{m} = \frac{abC}{(1+aC)}$ Adsorption constants:	Ward and Getzen, 1970

pka	pH of soln.	a*	b	x/m
3.92	3	0.431	645	630
	7	0.125	235	218
	11	0.100	59	54

Experimental conditions: 100 ml aqueous acid solution: 10 mg carbon

*Units: a = liters/μ mole
b = μ moles/g
c = μ moles/liter
$\frac{x}{m}$ = μ moles/g

TABLE 6: *Continued*

Compound Name	Adsorbent		Ref.
Alcohol *n*-butyl alcohol C_4H_9OH Compound properties m.w. 74.12[a] m.p. -90°C[a] b.p. 117-118°C[a]; 117.71°C[b] density 0.810_4^{20}[a] water sol 7.9 gm/100 ml[b]	Graphite Blood Char.	Adsorption equation: $\frac{x'}{m} = \frac{x}{m}(1+N_b\bar{v}_b/N_a\bar{v}_a)$ N = mole fraction $\bar{v}$ = partial molar volume a = solvent b = solute	Bartell, Thomas, and Fu, 1951

t°C	K*	ΔF°** kcal/mole	ΔH°*** kcal/mole
0	63.3	-2.24	-0.16
25	61.6	-2.43	-1.47
45	52.7	-2.50	
0	477	-3.34	-0.94
25	412	-3.54	-0.52
45	390	-3.76	

*Equilibrium constant K obtained from the limiting slope of the adsorption isotherms at zero concentration

**$\Delta F° = -RT \ln K$

***$\Delta H° = R\frac{(T_2T_1)}{(T_2-T_1)} \ln \frac{K_2}{K_1}$

TABLE 6: *Continued*

Compound Name	Ref.

Amides

acetanilide and derivatives, adsorption from 2% ethanol

C_8H_9ON

Compound properties[b]

m.w. 135.16

m.p. 114°C

b.p. 305°C

density 1.21^{4}_{4}

water sol 0.563^{25}; 3.5^{80}

Adsorption equation: $(\frac{x}{m}) = KC^{1/n}$

$1/n = 1$

Ward and Upchurch, 1965

Compound	solubility (x 10^{-4}M) 2% ethanol	k_N*	k_A**
N-Ethylacetanilide	2320	0.05	0.20
4-Hydroxyacetanilide	1580	0.25	0.13
Acetanilide	624	0.21	0.32
2-Chloroacetanilide	375	0.25	0.47
4-Aminoacetanilide	352	0.06	0.05
N-*n*-Butylacetanilide	167	0.23	0.89
2-Nitroacetanilide	138	0.16	0.72
2-Hydroxyacetanilide	32	0.26	0.15
N-Phenylacetanilide	31	0.26	1.59
4-Chloroacetanilide	16	1.19	2.64
3,4-Dichloroacetanilide	12	6.05	6.83
4-Nitroacetanilide	11	1.02	2.18
4-Bromoacetanilide	11	1.73	3.30
2,5-Dichloroacetanilide	10	0.92	1.59

Method of analysis: UV spectrophotometry with Beckman DU spectrophotometer

* k_N = adsorption on nylon

** k_A = adsorption on cellulose triacetate

TABLE 6: *Continued*

Compound Name	Ref.
aniline and derivatives, adsorption from 2% ethanol $C_6H_5NH_2$	Ward and Upchurch, 1965

Compound properties

m.w. 93.13^a

m.p. $-6.3°C^a$

b.p. $184.13°C^a$

density 1.02173_4^{20a}

water sol 3.4^{20}; 6.4^{90b}

Adsorption equation: $(\frac{x}{m}) = KC^{1/n}$; $1/n = 1$

Compound	solubility (x 10^4M) 2% ethanol	k_N*	k_A**
Aniline	4450	0.07	0.27
2-Methylaniline	1670	0.10	0.44
4-Methylaniline	1240	0.05	0.50
N-Methylaniline	560	0.24	0.92
4-Chloroaniline	520	0.68	3.31
2-Chloroaniline	450	0.55	1.94
N-Ethylaniline	250	0.32	1.10
2-Nitroaniline	103	0.91	2.84
N,*N*-Dimethylaniline	95	0.52	2.12
2,3-Dichloroaniline	85	3.45	7.20
3,4-Dichloroaniline	52	4.32	10.20
2,5-Dichloroaniline	49	3.78	11.20
4-Nitroaniline	38	1.10	3.40
N-*n*-Butylaniline	16	1.42	6.55
2-Nitro-4-chloroaniline	9	3.70	7.80
2,4-Dinitroaniline	5	1.94	5.65
N-Benzylaniline	4	3.46	19.48
N-Phenylaniline	3	16.50	24.00

Method of analysis: UV spectrophotometry with Beckman DU spectrophotometer.

*k_N = adsorption on nylon

**k_A = adsorption on cellulose triacetate

TABLE 6: *Continued*

Compound Name		Ref.
4-(R_2 sulfonyl)-2,6-dinitro-*N*,*N*-(di-R_1) aniline	Adsorption equation: $\ln K_e = aP\Delta U$*	Lambert, 1967

			K_e values	
SD	R_1	R_2	Ripperdan soil 1% O.m	Sacramento soil 5% O.m
11830	CH_3	CH_3	125	145
12639	C_2H_5	CH_3	230	193
11831	C_3H_7	CH_3	500	520
13207	C_2H_5	C_2H_5	320	269
12030	C_3H_7	C_2H_5	750	702
12346	C_3H_7	C_3H_7	1170	-
12400	CH_3	iso-C_3H_7	222	

*K_e = equilibrium constant, estimated from adsorption data

$P = \frac{m\gamma^{1/4}}{\rho}$, P = parachor, ρ = density of the liquid, γ = surface tension, M = molecular weight

ΔU = difference in internal pressures of the solvent phases

TABLE 6: *Continued*

Compound Name			Ref.
crystal violet (gentian violet) $C_{25}H_{30}ClN_3$ Compound properties[c] m.w. 408.06 water sol soluble	Adsorbent activated charcoal B10	Adsorption equation: $y= a\cdot x^b$ Adsorption constants:	Spahn et al. 1974

x-range I (mmol/dm^3	a	b
0.1 - 2	0.84	0.09

Compound Name			Ref.
Amino acid *dl*-tryptophan, from aqueous urea solution $C_{11}H_{12}N_2O_2$ Compound properties m.w. 204.22 m.p. 283-5°C water sol slightly sol cold sol hot	Adsorbent carbon black	Adsorption equation: $M= \frac{abC}{1+bC}$	Nogami, Nagai, and Uchida, 1968

Urea Concentration M	a 10^{-3} liter mole	b 10^{-3} liter mole	ΔF Kcal mole	ΔH Kcal mole	ΔS e.u.	ΔS_t e.u.	ΔS_s e.u.
0	1.63	1.70	-4.45	0.22	15.4	0	15.4
0.11	1.60	1.70	-4.45	--	15.4	0.05	15.4
1.01	1.54	1.08	-4.18	--	14.5	0.38	14.9
3.05	1.28	0.615	-3.87	--	13.5	1.15	14.7
5.03	1.18	0.472	-3.70	--	12.9	1.68	14.6
7.07	0.92	0.397	-3.57	--	12.5	2.08	14.6

ΔF = free energy change

ΔS = entropy change

$\Delta S_s = \Delta S + \Delta S_t$

ΔS_t = entropy change of the transfer of tryptophan from aqueous solution to aqueous urea solution

e.u. = entropy units

TABLE 6: *Continued*

Compound Name		Ref.
Benzene		
benzene - adsorption from binary mixture	Adsorption equation:	Zettlemoyer and Micale,
C_6H_6	$$\frac{X_1X_2}{n^{\circ}\Delta X/m} = \frac{1}{n^s}[X_1+\frac{1}{K-1}]$$	1971
Compound properties		
m.w. 78.11[d]		
density .87901[b]		
m.p. 5.5°C[e]		
b.p. 80.1°C[e]		
water sol 820 ppm at 22°C[f] OCT/water part coeff 130[g]		

Solvent	Adsorbent	K	Area of adsorbent m^2/g	$(\Delta H_1^{\circ} - \Delta H_2^{\circ}*)$ cal/g
Ethylene dichloride	Graphon	18.5	119	0.54
	Spheron 6	5	57	-
Cyclohexane	Coconut shell charcoal	19.9	677	12.0
	Decolorizing charcoal	16.4	596	7.1
Carbon tetrachloride	Decolorizing charcoal	16.1	374	4.0
	Coconut shell charcoal	18.2	350	3.8

$*\Delta H = X_1^S\Delta H_1^{\circ}+X_2^S\Delta H_2^{\circ}$

$K = \exp-(\frac{\Delta Ha}{RT} - \frac{\Delta Sa}{R})$

TABLE 6: *Continued*

Compound Name		Ref.
Carbamates		
carbamate derivatives, adsorption from 2% ethanol $R_1NHCOOR_2$	Adsorption equation: $(\frac{x}{m}) = KC^{1/n}$ $1/n = 1$	Ward and Upchurch, 1965

Compound	solubility 2% ethanol	k_N*	k_A**
Ethyl-*N*-methyl-*N*-phenyl	172	0.22	1.42
Ethyl-*N*-benzyl	121	0.49	2.03
Ethyl-*N*-phenyl	96	1.03	3.68
Ethyl-*N*-ethyl-*N*-phenyl	78	0.25	1.83
Ethyl-*N*-(2-nitrophenyl)	71	0.90	3.25
N-Phenylglycine ethyl ester	64	0.16	0.83
Phenyl	28	0.40	0.58
Isopropyl-*N*-phenyl	16	1.16	4.95
Ethyl-*N*-(4-chlorophenyl)	9.6	5.70	14.70
Ethyl-*N*-butyl-*N*-phenyl	8.5	0.80	6.75
n-Butyl-*N*-phenyl	8.5	2.20	9.62
Ethyl-*N*-(4-nitrophenyl)	5.7	3.65	8.75
Ethyl-*N*-benzyl-*N*-phenyl	2.9	1.85	12.65
Ethyl-*N*-(2,5-dichlorophenyl)	2.6	4.00	19.40
Ethyl-*N*-(2,3-dichlorophenyl)	2.5	3.65	27.90
Ethyl-*N*,*N*-diphenyl	1.7	1.02	9.10
Isopropyl-*N*-(2-methyl-5-chlorophenyl)	1.6	3.37	14.00
Methyl-*N*-(2,4-dichlorophenyl)	0.72	15.10	--
Isopropyl-*N*-(3-chlorophenyl)	0.50	9.00	8.45
Isopropyl-*N*-(3,4-dichlorophenyl)	0.32	23.00	--

Method of analysis: UV spectrophotometry with Beckman DU spectrophotometer

*k_N = (amount adsorbed/weight of nylon)/($C^{1/n}$)

**k_A = (amount adsorbed/weight of cellulose triacetate)/($C^{1/n}$)

TABLE 6: *Continued*

Compound Name	Ref.
carbamate derivatives, adsorption from 2% ethanol	Ward and Upchurch, 1965

Adsorption equation: $\frac{x}{m} = KC^{1/n}$ (1/n = 1)

Adsorbent	Compound	k_N		
		10°C	26.5°C	50°C
Nylon (Zytel-101) (80 mesh)	Ethyl-*N*-phenyl	1.03	1.03	1.03
	Isopropyl-*N*-phenyl	1.16	1.16	1.16
	Ethyl-*N*-methyl-*N*-phenyl	0.22	0.22	0.22
	Ethyl-*N*-ethyl-*N*-benzyl	0.25	0.25	0.25
	Ethyl-*N*-benzyl-*N*-phenyl	1.33	1.85	1.85
	Ethyl-*N*,*N*-diphenyl	0.66	1.02	1.02
	Isopropyl-*N*-(3-chlorophenyl)	9.00	9.00	9.00
	Ethyl-*N*-(2-nitrophenyl)	0.75	0.90	0.90
	Ethyl-*N*-(4-nitrophenyl)	3.65	3.70	3.70
	Ethyl-*N*-(2,3-dichlorophenyl)	3.70	3.70	3.70

Method of analysis: UV spectrophotometry with Beckman DU spectrophotometer.

TABLE 6: *Continued*

Compound Name			Ref.
Carbonyls			
acetophenone $C_6H_5COCH_3$	Adsorbent activated charcoal B 10	Adsorption equation: $y = a \cdot x^b$	Spahn et al., 1974
Compound properties m.w. 120.16[h] m.p. 20.5°C[h] b.p. 202.0°C[h] density 1.0281 at 20°C/4°C[h] water sol 5.6×10^{-3}M at 25°C[i]		Adsorption constants: x-range I (mmol/dm^3) — a — b 0.1 - 4 — 3.46 — 0.155	
N-Heterocyclics			
benzo[f]quinoline $C_{13}H_9N$		Adsorption equation: $S_s = K_p S_w$, n=1	Smith, Mabey, Bohonos, Holt, Lee, Chou, Bomberger, Mill, 1977
Compound properties m.w. 179.22 m.p. 93.5°C b.p. 350°C (721 torr) 202-5°C (8 torr) vapor pressure at 20°C (torr) water sol (μg ml^{-1}) 76.1±2.2	Adsorbent Coyote Creek sediment	TOC* — CEC** — Kp 1.4 — 13.5 — 1313±170	

*TOC - total organic carbon

**CEC - cation exchange capacity

TABLE 6: *Continued*

Compound Name					Ref.
9H-carbazole		Adsorption equation: $C_s = K_pC_w$			Smith, Mabey, Bohonos, Holt, Lee, Chou, Mill, Bomberger, 1977b
$C_6H_4NHC_6H_4$					
Compound properties	Adsorbent	Kp			
m.w. 167.21	Ca-montmorillonite	3.20±1.06			
m.p. 247-248°C	Coyote creek sediment	175 ±20.9			
water sol (1.0 μg/ml)					
7H-dibenzocarbazole (DBC)		Adsorption equation: $C_s = K_pC_w$			Smith, Mabey, Bohonos, Holt, Lee, Chou, Mill, Bomberger, 1977a
$C_{10}H_6NHC_{10}H_6$					
Compound properties	Adsorbent	TOC*	CEC**	K_p ***	
m.w. 267.31	Des Moines River sediment	0.8	10.5	32,600	
m.p. 155-159°C	Coyote Creek sediment	1.9	13.5	18,500	
water sol $2.4X10^{-7}M$	Searsville Lake sediment	5.0	34.5	27,600	

*TOC = total organic carbon

**CEC = cation exchange capacity

***Based on analysis of the supernatant at equilibrium

TABLE 6: *Continued*

Compound Name		Ref.
pyridine C_5H_5N Compound properties[j] m.w. 79.10 m.p. 42.0°C b.p. 115.3°C density .982 at 20°C water sol =	Adsorption equation: $y = a \cdot x^b$	Spahn et al., 1974
pyridine	Adsorption equation: $X = KCe^n$, X = mg/g; Ce = mg/l	Baker and Luh, 1971

Spahn et al., 1974:

Adsorbent	x-range I (mmol/dm^3)	a	b
activated charcoal B 10	0.14 - 7.4	1.22	0.2

Baker and Luh, 1971:

Adsorbent	Temp.	pH	K	n
Na-kaolinite	1°	2	0.03	1.01
	24°	2	0.01	1.03
Na-montmorillonite	1°	2	0.12	1.04*
	24°	2	0.06	1.02

Method of analysis: liquid scintillation with Packard Tri-Carb spectrometer

Note: clay: pyridine ratio was varied from 12.15 to 6.25×10^4
for ratio (12.15) effect of pH was studied:
max adsorption for Na-kaolinite was found at pH 5.5; pka pyridine = 5.25
max adsorption for Na-montmorillonite was found at pH 4.0

*discrepancy noted between data given Table 2 p.842 and regression equation p.843, believe this correct value.

TABLE 6: *Continued*

Compound Name		Ref.
quinoline C_9H_7N Compound properties m.w. 129.15 water sol 6.11 μg/ml $pK_b = 9.5$* m.p. -14.5°C b.p. 161.9°C	Adsorption equation: $K_p = \frac{\mu g \text{ adsorbed}}{g} / \frac{\mu g \text{ in solution}}{ml}$	Smith, Mabey, Bohonos, Holt, Lee, Chou, Mill, Bomberger, 1976b

Adsorbent	TOC	CEC	K_p
Ca-montmorillonite	0.05	69	7.28±0.52
Coyote Creek sediment	1.4	13.5	10.9±0.4

Experimental conditions: quinoline concentrations 4 and 8 $\mu g/ml^{-1}$; sediment concentrations 1000 to 3000 times that of quinoline.

Method of analysis: UV spectrophotometry with Cary Model 11 spectrophotometer.

*Quinoline is calculated to be 97%, 24%, and 0.32% protonated at pH 3, 5, and 7, respectively.

TABLE 6: *Continued*

Compound Name					Ref.
S-Heterocyclics					
benzo[*b*]thiophene					
C_8H_6S		Adsorption equation: $S_s=K_pS_w$, n=1			Smith, Mabey, Bohonos, Holt, Lee, Chou, Mill, Bomberger, 1976c
Compound properties	Adsorbent	TOC	CEC	K_p	
m.p. 31.3°C	Coyote Creek sediment	1.4	13.5	50±5	
b.p. 212.9°C					
water sol 127.3±2.5 at 20°C					
	Experimental conditions: sediment loadings of 2000:1 and 5000:1 sediment: BT by weight				
dibenzothiophene					
$C_{12}H_8S$		Adsorption equation: $S_s=K_pS_w$, n=1			Smith, Mabey, Bohonos, Holt, Lee, Chou, Bomberger, Mill, 1977
Compound properties	Adsorbent	Toc	CEC	K_p	
m.w. 184.27	Coyote Creek sediment	1.4	13.5	1380±130	
m.p. 99-100°C					
b.p. 332-333°C					
water sol 1.11±0.09					

TABLE 6: *Continued*

Compound Name	Adsorbent				Ref.
Phenols					
phenol		Adsorption equation: $y=a\cdot x^b$			Spahn et al.,
C_6H_5OH	Adsorbent				
Compound properties	activated charcoal B 10	X-range I (mmol/dm^3)	a	b	1974
m.w. 9411[d]		0.1-8	2.16	0.23	
m.p. 40.9°C[e]					
b.p. 180°C/740mm[k]		X-range II			
density 1.072 g/ml[b]		(mmol/dm^3)	a	b	
water sol 84.12 mg/ml[k]		0.001-0.06	3.6	0.39	
Polynuclear aromatics					
benz[*a*]anthracene		Adsorption equation: $s_s=K_pS_w$, n=1			Smith, Mabey, Bohonos, Holt, Lee, Chou, Bomberger, Mill,
$C_{18}H_{12}$					
Compound properties					
m.w. 228.28	Adsorbent	TOC	CEC	K_p	
m.p. 155-7°C	Coyote Creek sediment	1.4	13.5	26,200±1700	1977
b.p. (at 760 torr) 435°C					
water sol at 27°C					

TABLE 6: *Continued*

Compound Name		Ref

benz*o*[*a*]pyrene

$C_{20}H_{12}$

Compound properties

m.w. 252.32[a]

m.p. 178°C[l]

b.p. ~500°C[l]
311°C at 10 torr

water sol 1.2±0.1 ng/ml

Adsorption equation: $x=K_pC$

Adsorbent	Total organic carbon (%)	CEC meg. $100g^{-1}$	K_p $(x10^{-4})$
Ca-montmorillonite	0.06	69.0	1.7±0.5
Des Moines River	0.6	10.5	3.5±2.7
Coyote Creek	1.4	13.5	7.6±2.4
Searsville Pond	3.8	34.5	15.0±2.2

Ref: Smith, Mabey, Bohonos, Holt, Lee, Chou, Mill, Bomberger, 1976a

pyrene

$C_{16}H_{10}$

Compound properties

m.w. 202[l]

m.p. 150°C[l]

b.p. 393°C[e]

density 1.1271[a]

water sol .135±.005 mg/1[m]

Oct water part coeff:[g]
KOW=150,000

Adsorption equation: $\frac{c}{q} = \frac{1}{Kq^{\circ}} + \frac{c}{q^{\circ}}$

q = heat evolved when the [cyclohex] is c

q° = total heat evolved when complete

Equilibrium constants:

Adsorbent	Est. from the Langmuir isotherm*	Est. from heat of ads. data	ΔF** Kj/mole	ΔH Kj/mole
graphon	2200	1750	18.7	23
oleophilic graphite	5930	4800	21.1	18
"polar" graphite	2300	2340	18.9	26

Method of analysis: UV spectrophotometry with Unicam SP 500 spectrophotometer.

Ref: Groszek, 1975

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*at 21°

**ΔF° = -RTlnK

TABLE 6: *Continued*

Compound Name		Ref.
pyrene	Adsorption equation: $X=K_pC$; $KOC=K_p/OC$	Karickhoff, Brown, and Scott, 1979

Compound properties

water sol (mole fraction$\times 10^9$)=12

K octanol water=150,000

Adsorbent	% O.C.	K_p	KOC($\times 10^{-5}$)
Hickory Hill			
sand	0.13	42	0.32
coarse silt	3.27	3000	0.92
medium silt	1.98	2500	1.3
fine silt	1.34	1500	1.1
clay	1.20	1400	1.2
Doe Run			
sand	0.086	9.4	0.11
coarse silt	2.78	2100	0.76
medium silt	2.34	3000	1.3
fine silt	2.89	3600	1.2
clay	3.29	3800	1.2
Oconee River			
sand	0.57	68	0.12
coarse silt	2.92	3200	1.1
medium silt	1.99	2300	1.2
fine silt	2.26	2500	1.1
clay	-	-	-

Experimental conditions: sorbent concentrations 400 mg/ml of suspension for sand, 20 mg/ml for coarse and medium silt, 10 mg/ml for fine silt and 1 mg/ml for clay.

Method of analysis: UV spectrophotometry with Perkin Elmer 356 spectrophotometer.

TABLE 6: *Continued*

Compound Name	Adsorbent		Ref.
Quinone alizarin $C_{14}H_8O_4$ Compound properties[a] m.w. 240.23 m.p. 289-90°C (cor) b.p. 430°C (sub) water sol slightly sol	activated charcoal B 10	Adsorption equation: $y = a \cdot x^b$ Adsorption constants:	Spahn et al., 1974
Sulfonate sodium naphthalenesulfonate	Amberlite XAD-2	Adsorption equation: $\frac{C}{q} = \frac{1}{Kb} + \frac{C}{b}$ Method of analysis: UV spectrophotometry	Gustafson et al., 1968

Alizarin adsorption constants:

x-range I (mmol/dm^3)	a	b
0.1 - 8	1.39	0.095

Sodium naphthalenesulfonate:

t	K 1/mole	b mole/g	ΔH°* Kcal/mole	ΔFu°** Kcal	ΔSu°*** Kcal
25°C	319	4.58×10^{-5}	-4.4	-5.7	+4.4

*$\Delta H° = 2.303 \frac{RT_1T_2}{(T_2-T_1)} (\log K'_2 - \log K'_1)$

**$\Delta Fu° = RT\ln K$; $K = 55.5K$; $K = \theta/(1-\theta)C$; θ=fractional surface coverage

***$\Delta Su° = (\Delta H° - \Delta Fu°)/T$

TABLE 6: *Continued*

Compound Name	Ref.

PESTICIDES

Carbamates

carbaryl

N-methyl-1-naphthylcarbamate

$C_{12}H_{11}NO_2$

Compound properties[p]

m.w. 201

water sol 350 μmol/l

Desorption Equation: $K_b = P_s/P_w$

Adsorption Equation: $K_f = P_s/P_w$

LaFleur, 1976a

Adsorbent	pH	%o.m.	1/0.5	1/1	1/2	1/4	1/1
Lakeland s	5.3	0.22	0.44	0.21	0.16	0.13	
Norfolk ls	6.0	0.57	1.4	0.36	0.31	0.25	
Norfolk scl	5.4	0.15	0.72	0.12	0.10	0.08	
Cecil sl	6.3	1.77	5.2	1.8	1.6	1.3	0.79
Cecil c	5.7	0.53	0.88	0.27	0.22	0.19	
Okenee sl	4.65	5.16	7.6	3.7	2.6	2.3	

Method of analysis: UV spectrophotometry.

Chlorinated hydrocarbons

DDT

1,1'-(2,2,2-trichloroethylidene)-bis[4-chlorobenzene]

$C_{14}H_9Cl_5$

Compound properties

m.w. 354.49

Adsorption equation: $x/m = KC^{1/n}$

Huang and Liao, 1970

Adsorbent	K	1/n
illite	2.72×10^{-3}	3.28
kaolinite	7.37×10^{-6}	5.08
montmorillonite	1.10×10^{-5}	5.97

Method of analysis: GC - electron capture

TABLE 6: *Continued*

Compound Name | Ref.

dieldrin

1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-*endo*-1,4-*exo*-5,8-dimethanonaphthalene

$C_{12}H_8Cl_6O$

Compound properties

m.w. 380.91

Adsorption equation: $\frac{x}{m} = KC^{1/n}$

Huang and Liao, 1970

Adsorbent	K	1/n
illite	9.45×10^{-16}	8.82
kaolinite	1.46×10^{-21}	11.63
montmorillonite	1.05×10^{-16}	9.24

Method of analysis: GC-electron capture.

heptachlor

1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-4,7-methano-1*H*-indene

$C_{10}H_5Cl_7$

Adsorption equation: $\frac{x}{m} = KC^{1/n}$

Huang and Liao, 1970

Adsorbent	K	1/n
illite	1.09×10^{-9}	6.07
kaolinite	5.00×10^{-6}	4.51
montmorillonite	1.48×10^{-4}	3.52

Method of analysis: GC-electron capture.

TABLE 6: *Continued*

Compound Name					Ref.
methoxychlor					
$C_{16}H_{15}Cl_3O_2$	Adsorption equation: $X = K_pC$; $KOC = K_p/OC$				Karickhoff, Brown, and Scott,
Compound properties[a]	Adsorbent	% O.C.	K_p	KOC($X10^{-5}$)	1979
m.w. 345.65	Hickory Hill				
m.p. 78-78.2°C or 86-88°C	sand	0.13	53	0.41	
insol. in water	coarse silt	3.27	2600	0.80	
	medium silt	1.98	1800	0.91	
	fine silt	1.34	1400	1.0	
	clay	1.20	1100	0.92	
	Doe Run				
	sand	0.086	8.3	0.097	
	coarse silt	2.78	2200	0.80	
	medium silt	2.34	1700	0.73	
	fine silt	2.89	2300	0.80	
	clay	3.29	2400	0.73	
	Oconee River				
	sand	0.57	95	0.17	
	coarse silt	2.92	2500	0.86	
	medium silt	1.99	2000	1.0	
	fine sand	2.26	2100	0.93	
	clay	--	--	--	

Experimental conditions: sorbent concentrations 400 mg/ml of suspension for sand, 20 mg/ml for coarse and medium silt, 10 mg/ml for fine silt and 1 mg/ml for clay.

Method of analysis: UV spectrophotometry with Perkin Elmer 356 spectrophotometer.

TABLE 6: *Continued*

Compound Name					Ref
mirex			Adsorption equation: $S_s = K_p S_w$, n=1		Smith, Mabey, Bohonos, Holt, Lee, Chou, Bomberger, Mill,
$C_{10}Cl_{12}$					
Compound properties	Adsorbent	TOC	CEC	K_p	
m.w. 546.0					
m.p. 485 (decomp)	Coyote Creek sediment	1.4	13.5	460,000 ± 110,000	1977
vapor pressure at 50° torr 6×10^{-6}					
water sol at 22°C (pg/ml) 70±20					
Organophosphates					
aminoparathion			Adsorption equation: $x/m = KC_e^{1/n}$		Bowman and Sans,
$C_{10}H_{16}NO_3PS$					
O,O-diethyl *O-p*-aminophenyl phosphorothioate	Adsorbents	1/n	K		1977
Compound properties	Na-montmorillonite*	0.954	46.3		
m.w. 261.3	Ca-montmorillonite*	1.151	43.3		
water sol 390.0 µg/ml	Fe-montmorillonite*	>99.9% adsorption			
	Experimental conditions: 450 mg clay in 30 ml aqueous insecticide solution				
	Method of analysis: GC - alkali flame ionization detector				

*Prepared from Wyoming bentonite, < 2 µm fraction

TABLE 6: *Continued*

Compound Name				Ref.
fenitrothion				
O,O-dimethyl *O*-(3-methyl-4-nitrophenyl) phosphorothioate	Adsorption equation: $\frac{x}{m} = KC_e^{1/n}$			Bowman and Sans, 1977
$C_9H_{12}NO_5PS$				
Compound properties	Adsorbent	1/n	K	
m.w. 277.2	Na-montmorillonite*	1.163	71.1	
b.p. 118°C	Ca-montmorillonite*	1.952	64.0	
density 1.3227^{25}_{4}	Fe-montmorillonite*	1.773	740.1	
water sol 25.4 μg/ml				
	Experimental conditions: same as for aminoparathion.			
	Method of analysis: GC-alkali flame ionization detector.			
methyl parathion				
O,O-dimethyl *O-p*-nitrophenyl phosphorothioate	Adsorption equation: $\frac{x}{m} = KC_e^{1/n}$			Bowman and Sans, 1977
$C_8H_{10}NO_5PS$				
Compound properties	Adsorbent	1/n	K	
m.w. 263.2	Na-Montmorillonite*	1.032	65.4	
m.p. 37-38°C^{c}	Ca-Montmorillonite*	1.663	56.3	
density 1.358^{20}_{4}^{c}	Fe-Montmorillonite*	1.463	147.3	
water sol 45.0 μg/ml 50 ppm^{c}	Experimental conditions: same as for aminoparathion.			
	Method of analysis: GC-alkali flame ionization detector.			

*Prepared from Wyoming bentonite <2 μm fraction.

TABLE 6: *Continued*

Compound Name		Ref.
methyl parathion *O,O*-dimethyl *O-p*-nitrophenyl phosphorothioate $C_8H_{10}NO_5PS$ Compound properties m.w. 263.12	Adsorption equation: $K_p[\frac{\mu g\ \text{substate in solution}}{\text{ml solution}}]^{1/n}$ $n = 1.0$	Smith, Mabey, Bohonos, Holt, Lee, Mill, Bomberger, 1976

Sediment	K_p	95% confidence limit
Ca-montmorillonite	46.1	±2.2
Coyote Creek	50.6	±4.5
	55.0	±6.8
Searsville Pond	60.3	±3.5
Navarro River	47.6	±3.2
Des Moines River	41.6	±2.0
Oconee River	23.6	±1.3

Experimental conditions: methyl parathion concentrations at 4 and 8 μg/ml. Sediment concentrations were 1000 to 2000 times as concentrated as methyl parathion at 8 μg/ml and 1000 to 3000 times as concentrated as MP at 4 μg/ml.

TABLE 6: *Continued*

Compound Name		Ref
parathion	Adsorption equation: $x/m = KC^{1/n}$ or $\log x/m = \log K + 1/n \log C$	Wahid and Sethunathan, 1978

Adsorbent Soil No.*	pH	Soil organic matter, %	CEC	Natural K	Soils 1/n	Oxidized K	Soils 1/n
10	6.20	0.75	18.6	7.67	1.04		
8	6.25	1.62	26.6	12.30	1.05	3.16	1.33
11	6.30	2.88	42.8	38.02	1.11	10.72	1.33
13	5.20	5.52	19.2	125.90	1.05		
15	3.50	8.21	21.2	213.80	1.03		
14	3.30	24.62	28.9	457.10	1.02		

Experimental conditions: 1 g soil in 10 ml aqueous parathion solution

Method of analysis: liquid scintillation

amitrole

3-amino-1,2,4-triazole

$C_2H_4N_4$

pKa = 4.14 ($3\text{-ATH}^+ = H^+ + 3\text{-AT}$)

Compound properties

water sol 28 g/100 ml (23°C)

Adsorption equation: $X = X_m bC/(1+bC)$ — Nearpass, 1969

Adsorbent	X_m	b**
H sat. organic matter	63 mM/100g	0.015
Al sat. organic matter	49 mM/100g	0.010

Experimental conditions: 20:1 water to organic matter

Method of analysis: liquid scintillation

*all soils from India
**calculated from figure 2

TABLE 6: *Continued*

Compound Name		Ref.
s-Triazine		
cyanazine		
2-[[4-chloro-6-(ethylamino)-*s*-triazin-2-yl]amino]-2-methylpropionitrile	Adsorption equation: $\frac{x}{m} = KC^{1/n}$ Chromatography thin-layer (soil)	Majka and Lavy, 1977
$C_9H_{13}ClN_6$		

Adsorbents	pH	% o.m.	CEC	K	1/n	Rf
Monona silty clay loam (Typic Hapludoll)	6.5	2.9	21.2	4.6	0.96	0.39
Valentine loamy fine sand (Typic Ustipsamment)	6.6	1.4	10.1	3.4	0.86	0.74

Experimental conditions: 1 g soil with cyanazine added in 0.2 ml methanol: 10 ml water.

Method of analysis: liquid scintillation with Packard 3320 spectrometer.

TABLE 6: *Continued*

Compound Name											Ref
prometryne											LaFleur, 1976b
$C_{10}H_{19}N_5S$					Desorption $K_b = \frac{P_s}{P_w}$						
2,4-bis(isopropylamino)-6-methylthio-1,3,5-triazine	Adsorbent	pH	%O.M	CCC*	1/0.5	1/1	1/2	1/4	ΔG_{sp}** (Kcal/mol)	K_o(calc)***	
Compound properties	Lakeland s	5.3	0.22	3.0	1.5	0.86	0.74	0.67	-4.1	1060	
m.w. 241	Norfolk ls	6.0	0.57	6.5	2.1	1.5	1.2	1.0	-4.1	990	
water sol 200 μM/l at 20°C	Norfolk scl	5.4	0.15	28	5.7	3.4	2.6	2.3	-3.6	420	
	Cecil sl	6.3	1.77	15	7.9	4.0	3.2	2.8	-4.1	1110	
pKa = 4.05	Cecil c	5.7	0.53	18	3.7	2.3	1.7	1.6	-3.3	280	
	Okenee sl	4.65	5.16	19	19	12	9.0	7.0	-4.6	2340	

Method of analysis: UV spectrophotometry

*Cation combining capacity - methylene blue adsorption at pH5.

**$\Delta G_{sp} = -RT\ln k_o$

***$K_o = P_a/P_w$ P_a is P_s adjusted to soil weight

TABLE 6: *Continued*

Compound Name | Ref.

Urea

diuron

3-(3,4-dichlorophenyl)-1,1-dimethylurea

$C_9H_{10}Cl_2N_2O$

Compound properties^c

m.w. 233.10

m.p. 158-159°C

water sol 42 ppm at 25°C

Adsorption equation: $\frac{x}{m} = KC^{1/n}$

Chromatography thin-layer (soil)

Adsorbents	pH	% o.m.	CEC	K	1/n	R_f
Monona silty clay loam (Typic Hapludoll)	6.5	2.9	21.2	14.3	0.77	0.18
Valentine loamy fine sand (Typic Ustipsamment)	6.6	1.4	10.1	6.5	0.74	0.39

Experimental conditions: same as for cyanazine.

Method of analysis: liquid scintillation with Packard 3320 spectrometer.

Ref.: Majka and Lavy, 1977

fluometuron

1,1-dimethyl-3-(α,α,α-trifluoro-*m*-tolyl)urea

$C_{10}H_{11}F_3N_2O$

Compound properties^c

m.w. 232.21

m.p. 163-164°C

water sol 80 ppm at 25°C

Chromatography thin-layer (soil)

Adsorbent	% o.m.	CEC	pH	R_f
Bethony silt loam	4.4	12.4	6.3	0.57
Hector loam	4.8	9.2	6.3	0.65
Eufaula sand	0.3	0.6	6.7	0.98

Experimental conditions: 10 g soil: 10 ml of 0.01 N $CaCl_2$ solution containing 1,2,4, or 8 ppm fluometuron.

Method of analysis: liquid scintillation.

Ref.: Chang and Stritzke, 1977

TABLE 6: *Continued*

Compound Name		Ref.
tebuthiuron *N*-[5-(1,1-dimethyl)ethyl]-1,3,4-thiadiazol-2-yl-*N*,*N*'-dimethylurea $C_9H_{16}N_4OS$ Compound properties water sol 2500 μg/ml	Chromatography thin-layer (soil) Water solvent	Chang and Stritzke, 1977

Adsorbent	% o.m.	CEC	pH	R_f
Bethony silt loam	4.4	12.4	6.3	0.58
Hector loam	4.8	9.2	6.3	0.66
Eufaula sand	0.[illegible]	0.6	6.7	0.98

Experimental conditions: 10 gm of soil: 10 ml of 0.01 N $CaCl_2$ solutions containing 1,2,4, or 8 ppm tebuthiuron.

Method of analysis: liquid scintillation.

TABLE 6: *Continued*

Compound Name		Ref.
paraoxon		
O,O-diethyl *O-p*-nitrophenyl phosphate	Adsorption equation: $\frac{x}{m} = KC_e^{1/n}$	Bowman and Sans, 1977
$C_{10}H_{14}NO_6P$		

Compound properties

m.w. 275.2

water sol 3,250.0 μg/ml

Adsorbent	1/n	K
Na-Montmorillonite*	1.157	53.7
Ca-Montmorillonite*	1.449	42.9
Fe-Montmorillonite*	1.376	81.7

Experimental conditions: same as for aminoparathion.

Method of analysis: GC-alkali flame ionization detector.

Compound Name		Ref.
parathion		
O,O-diethyl *O-p*-nitrophenyl phosphorothioate	Adsorption equation: $\frac{x}{m} = KC_e^{1/n}$	Bowman and Sans, 1977
$C_{10}H_{14}NO_5PS$		

Compound properties

m.w. 291.3

m.p. 6.1[a]

b.p. 375°C[a]

density 1.2704_{20}^{20}[a]

water sol 12.9 μg/ml

Adsorbent	1/n	K
Na-Montmorillonite*	1.042	119.6
Ca-Montmorillonite*	1.513	120.8
Fe-Montmorillonite*	1.194	605.8

Experimental conditions: same as for aminoparathion.

Method of analysis: GC-alkali flame ionization detector.

*Prepared from Wyoming bentonite, <2 μm fraction.

NOTES, TABLE 6

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TABLE 7: AVERAGE VALUES OF ADSORPTION CONSTANTS FOR ORGANIC PESTICIDES[†]

Compound Name	Average* $1/n \pm S\%$	Average* $K \pm S\%$	Soils (No.)	Average** $K_d \pm S\%$	Average*** $K_{oc} \pm S\%$	Soils (No.)
S-triazines						
simazine	0.820±3.48		6	1.93±6.69	135±6.33	174
6-chloro-*N*,*N'*-diethyl-1,3,5-triazine-2, 4-diamine				16.3±30	159±5.66	2
$C_7H_{12}ClN_5$						
m.w. 201.66[a]						
propazine	0.95±1.7	2.68±33.0	4	2.37±7.06	160±11.6	54
2-chloro-4,6-bis (isopropylamino)-*s*-triazine				26.7±9.71	152±3.7	17
$C_9H_{16}ClN_5$						
m.w. 229.71[a]						

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$$*K = \frac{C_s}{C_w^{1/n}}$$

$$**K_d = \frac{C_s}{C_w}$$

$$***K_{oc} = \frac{X/m(\mu g/g \text{ of organic carbon})}{C_{eq}} = \frac{K_d(\mu g/g \text{ of soil})}{\% \text{ organic carbon}}$$

Value given is average of K and K_d adjusted for organic carbon

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}±S%	Soils (No.)
atrazine	0.772±8.65		19	2.94±10.8	172±6.42	79
6-chloro-*N*-ethyl-*N'*-(1-methylethyl)-1,3,5-triazine-2,4-diamine	0.709±10.7		6	25.5±20.4	102±5.80	24
$C_8H_{14}ClN_5$						
m.w. 215.69[a]						
prometone	0.81±2.1	3.65±26	4	3.31±16.5	300±19.5	49
2,4-bis(isopropylamino)-6-methoxy-*s*-triazine				13.1±11.5	73.8±5.1	15
$C_{10}H_{19}N_5O$						
m.w. 225.30[a]						
ametryne						
N-ethyl-*N'*-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine				6.17±11.1	380±10.0	33
				167.4	802	1
$C_9H_{17}N_5S$						
m.w. 227.33[a]						
prometryne	0.855±1.1	7.83±31	4	7.03±8.78	513±13.0	53
2,4-bis(isopropylamino)-6-(methylthio)-*s*-triazine	1.76	50.3	1	55.8±8.46	311±5.12	18
$C_{10}H_{19}N_5S$						
m.w. 241.36[a]						

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** $K_d \pm S\%$	Average*** $K_{oc} \pm S\%$	Soils (No.)
ipazine				47.7	2571	1
6-chloro-*N*,*N*-diethyl-*N'*-(1-methylethyl)-1,3,5-triazine-2,4-diamine						
$C_{10}H_{18}ClN_5$						
m.w. 243.74[a]						
hydroxyatrazine				51.5	888	1
G30026	0.702	37.4			81.8	
Norazine						
$C_7H_{12}ClN_5$						
m.w. 201.66[a]						
Ureas and Uracils						
Urea	0.717	5.22			14.3	1
CH_4N_2O						
Compound properties[b]						
density 1.32_4^{18}						
m.w. 60.06						
m.p. 132.7°C						

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}±S%	Soils (No.)
fenuron	0.953±0.95	0.554±20.6	3	0.781±17.0	0.554±20.6	13
N,N-dimethyl-*N'*-phenylurea; 1,1-dimethyl-3-phenylurea	1.01±3.20	6.22±35.3	3	1.01±3.2	0.622±35.3	1
$C_9H_{12}N_2O$						
m.w. 164.21[a]						
methylurea	0.604±2.38	1.73±26.3	3		70.2±7.59	
	0.832±4.71	12.5±48.3	3		57.6±8.43	
phenylurea	0.744±1.34	1.80±14.8	3		76.7±8.83	
$C_7H_8N_2O$	0.733±2.90	21.7±52.9	3		98.3±12.9	
Compound properties[b]						
m.w. 136.15						
density 1.302						
m.p. 147°C						
b.p. 238°C						
bromacil	0.58, 0.85	0.08, 1.5	2	19, 123		
5-bromo-6-methyl-3-(1-methylpropyl)-uracil						
$C_9H_{13}BrN_2O_2$						
Compound properties[b]						
m.w. 261.11						
m.p. 157.5-160°C						

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}±S%	Soils (No.)
terbacil	0.50, 0.96	0.15, 1.7	2		37, 140	
5-chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1*H*,3*H*)-pyrimidinedione						
$C_9H_{13}ClN_2O_2$						
m.w. 216.67[a]						
monuron	0.74	5.98	1	2.17±18.9	83.1±22.9	31
N'-(4-chlorophenyl)-*N*,*N*-dimethylurea	0.83	23.6	1	33.3±22.3	163±16.7	6
$C_9H_{11}ClN_2O$						
Compound properties[b]						
m.w. 198.65						
m.p. 170.5-171.5°C						
water sol 230 ppm at 25°C						
diuron	0.818±6.45		10	6.29±9.33	351±8.95	79
3-(3,4-dichlorophenyl)-1,1-dimethylurea	0.707±5.10		3	196±39.2	902±31.9	4
$C_9H_{10}Cl_2N_2O$						
Compound properties[b]						
m.w. 233.10						
water sol 42 ppm at 25°C						

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}±S%	Soils (No.)
metobromuron					60±20	4
3-(*p*-bromophenyl)-1-methoxy-1-methylurea						
$C_9H_{11}BrN_2O_2$						
m.w. 259.11[a]						
chlorobromuron					217±20	4
monolinuron	0.810±0.302	9.24±9.75	3	9.24±9.75	195±38.9	7
3-(4-chlorophenyl)-1-methoxy-1-methylurea	0.832±2.33	43.0±48.5	3	43.0±48.5	198±8.67	3
$C_9H_{11}ClN_2O_2$						
m.w. 214.65[a]						
neburon	0.956±2.51	27.9±53.4			787±6.89	3
1-butyl-3-(3,4-dichlorophenyl)-1-methylurea						
$C_{12}H_{16}Cl_2N_2O$						
m.w. 275.18						
linuron	0.75, 0.75	45.2, 67.8	2	18.1±18.7	840±20	26
N'-(3,4-dichlorophenyl)-*N*-methoxy-*N*-methylurea				147±77.2	653±13.4	3
$C_9H_{10}Cl_2N_2O_2$						
Compound properties[b]						
m.w. 249.10						
m.p. 93-94°C						
water sol 75 ppm						

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}±S%	Soils (No.)
Halogenated Hydrocarbons						
ethylene dibromide	0.967, 0.970	0.408, 0.803	2	0.537±24.8	32.4±23.7	3
1,2-dibromoethane	1.04	2.16	1	2.13±1.41	14.4±19.4	2
$C_2H_4Br_2$						
m.w. 187.87[a]						
beta-BHC	0.861	148	1		4254	
1,2,3,4,5,6-hexachlorocyclohexane						
$C_6H_6Cl_6$	0.950	456	1		3573	
m.w. 290.85[a]						
lindane	0.841,080	45.7, 7.91	2	24.7±27.8	1342±15.3	6
1α,2α,3β,4α,5α,6β-hexachlorocyclohexane	0.981	331	1	321±6.10	1943±20.4	4
$C_6H_6Cl_6$						
Compound properties[b]						
m.w. 290.85						
m.p. 112.5°C						
insol. in water						

TABLE 7: *Continued*

Compound Name	Average* $1/n \pm S\%$	Average* $K \pm S\%$	Soils (No.)	Average** $K_d \pm S\%$	Average*** $K_{oc} \pm S\%$	Soils (No.)
N-serve				6.80±30.1	271±11.5	9
2-chloro-6-(trichloromethyl)-pyridine				44.5	238	1
$C_6H_3Cl_4N$						
Compound properties[b]						
m.w. 230.93						
m.p. 62.5-62.9°C						
b.p. 136-137.5°C						
DDT				$1.3X10^5$, $1.37X10^4$	$1.31X10^5$ $3.55X10^5$	2
				$1.063X10^5$	$2.29X10^5$	1
Carbamates						
chloropropham	1.00	21	1	9.28±11.8	590±8.35	65
isopropyl-*m*-chlorocarbanilate	1.00	132	1			
$C_{10}H_{12}ClNO_2$						
m.w. 213.67[a]						
propham					51	4
isopropyl carbanilate						
$C_{10}H_{13}NO_2$						
m.w. 179.22[a]						

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}±S%	Soils (No.)
EPTC				5.96±24.6	283±18.9	3
S-ethyl dipropylcarbamothioate				52.6	109	1
$C_9H_{19}NOS$						
m.w. 189.32[a]						
cycloate				7.32±25	345±17.4	3
S-ethyl cyclohexylethylcarbamothioate				66.6	222	1
$C_{11}H_{21}NOS$						
m.w. 215.36[a]						
pebulate				14.5±20.1	719±21.4	3
S-propyl butylethylthiocarbamate				109	363	1
$C_{10}H_{21}NOS$						
m.w. 203.35[a]						

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}±S%	Soils (No.)
Phosphates						
nellite				0.525±72.5	30.89±25.9	8
$C_8H_{13}N_2O_2P$				6.30, 6.02	43.5, 33.2	2
m.w. 200.18[a]						
crotoxyphos				6.09±15	173±34	3
(E)-1-phenylethyl-3-[(dimethoxyphosphinyl)oxy]-2-butenoate						
$C_{14}H_{19}O_6P$						
m.w. 314.28[a]						
phorate	0.97±2.1	8.76±39	4		3199±25	
O,O-diethyl *S*-[(ethylthio) methyl] phosphorodithioate						
$C_7H_{17}O_2PS_3$						
m.w. 260.38[a]						

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}±S%	Soils (No.)
disulfoton	0.930±2.38	20.1±18.9	10		2132±25	16
O,O-diethyl *S*-[2-(ethylthio)ethyl] phosphorodithioate						
$C_8H_{19}O_2PS_3$						
Compound properties[b]						
m.w. 274.41						
b.p. 108°C						
density 1.144_4^{20}						
insol. in water						
methyl parathion	1.04	18.43±20	4		9799±41	
O,O-dimethyl *O*-(4-nitrophenyl) phosphorothioate						
$C_8H_{10}NO_5PS$						
Compound properties[b]						
m.w. 263.23						
m.p. 37-38°C						
density 1.358_4^{20}						
water sol 50 ppm						
parathion	1.03±1.5	2.19±32	4		10454±38	
O,O-diethyl *O*-(4-nitrophenyl) phosphorothioate						
$C_{10}H_{14}NO_5PS$						
m.w. 291.26						

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}± S%	Soils (No.)
ethion *0,0,0',0'*-tetraethyl *S,S'*-methylenebisphosphorodithioate $C_9H_{22}O_4P_2S_4$ Compound properties[b] m.w. 384.48 m.p. -12 to -13°C density 1.220$^{20}_{4}$ slightly sol in water	0.945±2.5	28.5±15.9	4		15435±39.3	
carbophenothion *S*-[[(4-chlorophenyl)thio]methyl] *0,0*-diethyl phosphorodithioate $C_{11}H_{16}ClO_2PS_3$ Compound properties[b] m.w. 342.85 b.p. 82°C density 1.271$^{25}_{4}$ insol. in water	0.940±3.7	74.5±13	4		45368±40.6	

TABLE 7: *Continued*

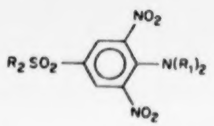
Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}±S%	Soils (No.)
Amino, Nitrophenyl Sulfones						
						
nitralin ($R_1 = CH_3H_7$; $R_2 = CH_3$) 4-(methylsulfonyl)-2,6-dinitro-N,N-dipropylbenzenamine $C_{13}H_{19}N_3O_6S$ m.w. 345.38				50, 26	500, 520	2
SD11830 ($R_1 = CH_3$; $R_2 = CH_3$)				12.5, 7.25	125, 145	2
SD12639 ($R_1 = C_2H_5$; $R_2 = CH_3$)				23, 9.65	230, 193	2
SD13207 ($R_1 + C_2H_5$; $R_2 = C_2H_5$)				32, 13.5	320, 269	2
SD12030 ($R_1 = C_3H_7$; $R_2 = C_2H_5$)				75, 35.1	750, 702	2
SD12346 ($R_1 = C_3H_7$; $R_2 = C_3H_7$)				117	1170	2
SD12400 ($R_1 = CH_3$; $R_2 = C_3H_7$)				22.2	222	2

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}±S%	Soils (No.)
Carboxylic Acids						
dicamba				0.9	3.8	1
3,6-dichloro-2-methoxybenzoic acid						
$C_8H_6Cl_2O_3$						
m.w. 221.04[a]						
chloramben NH_4^+ salt				0.320±30.4	15.4±37	9
chloramben: 3-amino-2,5-dichlorobenzoic acid				4.1	17.4	1
$C_7H_5Cl_2NO_2$						
m.w. 206.03[a]						
chloramben methyl ester				3.5±35	507±24	4
MCPA				0.420±37.4		
(4-chloro-2-methylphenoxy)-acetic acid						
$C_9H_9ClO_3$						
m.w. 200.62						

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}±S%	Soils (No.)
picloram 4-amino-3,5,6-trichloro-2-pyridinecarboxylic acid $C_6H_3O_2Cl_3N_2$ m.w. 241.46[a]				0.453±32.2	12.7±21.7	14
2,4-D (2,4-dichlorophenoxy)-acetic acid $C_8H_6Cl_2O_3$ m.w. 221.04[a]				1.59±54.9		7
2,4,5-T (2,4,5-trichlorophenoxy)-acetic acid $C_8H_5Cl_3O_3$ m.w. 255.49[a]				1.05±42.3		7
dichlobenil		167		4.19±11.4	164±3.57	16

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}±S%	Soils (No.)
Acids						
linear alkyl				34.2±57.4	1222±10.2	30(K_d) 20(K_{oc})
sulfonates				55.3	170	1
pentachlorophenol				8.96±20.38		10
C_6HCl_5O						
Compound properties[b]						
m.w. 266.35						
m.p. 190-191°C						
b.p. 309-310°C						
density 1.978^{22}_{4}						
water sol. 8 mg/100 ml						
methane arsonate				12.4±38.9	770±19.1	4
CH_5AsO_3						
Compound properties[b]						
m.w. 139.96						
m.p. 161°C						
freely sol. in water						

TABLE 7: *Continued*

Compound Name	Average* 1/n±S%	Average* K±S%	Soils (No.)	Average** K_d±S%	Average*** K_{oc}±S%	Soils (No.)
Miscellaneous						
silvex	0.639, 0.987	42.1, 34.2	2		2786, 4682	
2-(2,4,5-trichlorophenoxy)-propionic acid	1.05	162	1		440	
$C_9H_7Cl_3O_3$						
Compound properties[b]						
m.w. 269.53						
m.p. 181.6°C						
0.014% sol. in water at 25°C						
chlorthiamid	0.868±1.28	4.72±8.13	5		107.2±6.42	
2,6-dichlorobenzene carbothioamide						
$C_7H_5Cl_2NS$						
chloroneb	1.3	20	1		1159	
1,4-dichloro-2,5-dimethoxy-benzene						
$C_8H_8Cl_2O_2$						
m.w. 207.06[a]						
paraquat	0.566±19.6	353±97			20152±65	
1,1'-dimethyl-4,4'-bipyridinium	0.360±13.3	5501±16.6				
$C_{12}H_{14}N_2$						
m.w. 186.26[a]						

NOTES, TABLE 7

[a] Wiswesser, W.J., ed. 1976. *Pesticide Index*. 5th ed. College Park, Maryland: The Entomological Society of America.

[b] Windholz, M., S. Budavari, L.Y. Stroumtsos, and M.N. Fertig. 1976. *The Merck Index*. 9th ed. Rahway, N.J.: Merck and Co.

TABLE 8: RELATIONSHIP BETWEEN OCTANOL/WATER PARTITION COEFFICIENT AND R_f VALUES OF PESTICIDES ON A SOIL

Mobility Class	R_f	log P*	Ω**	Ref
Immobile	0 - 0.09	>3.78	>398	Briggs, 1973
Low	0.10 - 0.34	3.78-2.39	398-74	
Intermediate	0.35 - 0.64	2.39-1.36	74-29	
Mobile	0.65 - 0.89	1.36-0.08	29-4.5	
Very Mobile	0.90 - 1.00	<0.08	<4.5	

* P = Octanol/water partition coefficient

** Ω = Soil organic matter/water partition coefficient

TABLE 9: LEACHING OF PESTICIDES FROM A SOIL

Compound Name				Ref.
Adsorbent = Hagerstown silty clay loam %O.M = 2.41, %O.C = %O.M/1.724 = 1.40				Hamaker, 1974
Pesticide	R_f (soil TLC)	Mobility class	K_{oc}*	
chloramben	0.96	5	12.8	
2,4-D	0.69	4	32	
propham	0.51	3	51	
bromacil	0.69	4	71	
monuron	0.48	3	83	
simazine	0.45	3	135	
propazine	0.41	3	152	
dichlobenil	0.22	2	164	
atrazine	0.47	3	172	
chlorpropham	0.18	2	245	
prometone	0.60	3	300	
ametryne	0.44	3	380	
diuron	0.24	2	485	
prometryne	0.25	2	513	
chloroxuron	0.09	1	4,986	
paraquat	0.00	1	20,000	
DDT	0.00	1	243,000	

*K_{oc} = adsorption coefficient on the basis of organic carbon

TABLE 10: SORPTION DEPENDENCE ON SORBATE PROPERTIES

Compound Name	Compound Properties			Ref.
Compound	Water solubility (mole fraction x 10^9)	$K_{oc}(X10^{-3})$*	$K_{ow}(X10^{-3})$**	
pyrene	12	84	150	Karickhoff, Brown, and Scott, 1979
methoxychlor	6.3	80	120	
naphthalene	4460	1.3	2.3	
2-methylnaphthalene	3220	8.5	13	
anthracene	7.57	26	35	
9-methylanthracene	24.4	65	117	
phenanthrene	130	23	37	
tetracene	0.037	650	800	
hexachlorobiphenyl	0.048	1200	2200	
benzene	189,000	0.083	0.13	

*K_{oc} = partition coefficient based on organic carbon

**K_{ow} = octanol/water distribution coefficient

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OCCURRENCE AND DISTRIBUTION OF ENERGY-RELATED ORGANIC COMPOUNDS

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APPENDIX: FORMULAS OF ORGANIC COUMPOUNDS

COMPOUNDS OTHER THAN PESTICIDES

Acids, Aliphatic

acetic acid

CH_3COOH

adipic acid

$HOOCCH_2CH_2CH_2CH_2COOH$

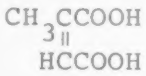
butyric acid

$CH_3CH_2CH_2COOH$

caproic acid

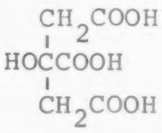
$CH_3CH_2CH_2CH_2CH_2COOH$

citraconic



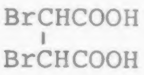
$$\begin{array}{l} CH_3CCOOH \\ \quad\;\, \| \\ \quad\;\, HCCOOH \end{array}$$

citric acid



$$\begin{array}{l} \quad\; CH_2COOH \\ \quad\;\, | \\ HOCCOOH \\ \quad\;\, | \\ \quad\; CH_2COOH \end{array}$$

dibromosuccinic

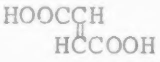


$$\begin{array}{l} BrCHCOOH \\ \quad\;\, | \\ BrCHCOOH \end{array}$$

formic acid

$HCOOH$

fumaric acid

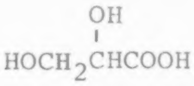


$$\begin{array}{l} HOOCCH \\ \qquad\;\; \| \\ \qquad\; HCCOOH \end{array}$$

glutaric acid

$HOOCCH_2CH_2CH_2COOH$

glyceric acid



$$\begin{array}{l} \qquad\qquad OH \\ \qquad\qquad\; | \\ HOCH_2CHCOOH \end{array}$$

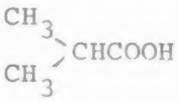
glycolic acid

$HOCH_2COOH$

glyoxylic acid

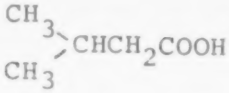
$HCOCOOH$

isobutyric acid



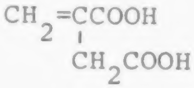
$$\begin{array}{l} CH_3 \\ \quad\; \rangle CHCOOH \\ CH_3 \end{array}$$

isovaleric acid



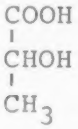
$$\begin{matrix} CH_3 \searrow \\ CHCH_2COOH \\ CH_3 \nearrow \end{matrix}$$

itaconic acid



$$\begin{array}{l} CH_2{=}CCOOH \\ \phantom{CH_2{=}}| \\ \phantom{CH_2{=}}CH_2COOH \end{array}$$

lactic acid

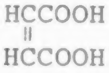


$$\begin{array}{l} COOH \\ | \\ CHOH \\ | \\ CH_3 \end{array}$$

levulinic acid

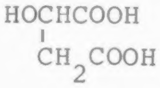
$CH_3COCH_2CH_2COOH$

maleic acid



$$\begin{array}{l} HCCOOH \\ \| \\ HCCOOH \end{array}$$

malic acid

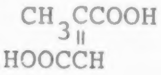


$$\begin{array}{l} HOCHCOOH \\ | \\ CH_2COOH \end{array}$$

malonic acid

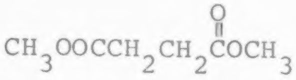
$HOOCCH_2COOH$

mesaconic acid



$$\begin{array}{r} CH_3CCOOH \\ \| \\ HOOCCH \end{array}$$

methylsuccinic acid



$$CH_3OOCCH_2CH_2\overset{\overset{O}{\|}}{C}OCH_3$$

monobromosuccinic

$HOOCCH_2CHBrCOOH$

oxalic

$HOOCCOOH$

propionic acid

CH_3CH_2COOH

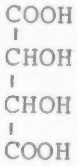
pyruvic acid

$CH_3COCOOH$

succinic acid

$HOOCCH_2CH_2COOH$

tartaric acid



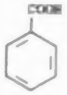
$$\begin{array}{l} COOH \\ | \\ CHOH \\ | \\ CHOH \\ | \\ COOH \end{array}$$

valeric acid

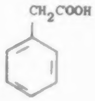
$CH_3CH_2CH_2CH_2COOH$

Acids, Aromatic

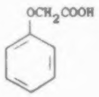
benzoic acid



phenylacetic acid



phenoxyacetic acid



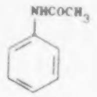
Alcohol

n-butyl alcohol

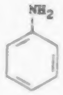
$CH_3CH_2CH_2CH_2OH$

Amines and derivatives

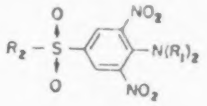
acetanilide



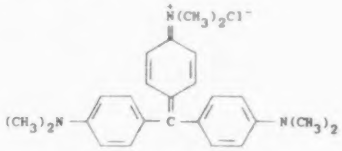
aniline



4-(R_2 sulfonyl)-2,6-dinitro-N.N.-(di-R_1)aniline

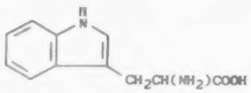

O
NO2
R2 – S
N(R1)2
O
NO2

crystal violet

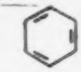

N⁺(CH3)2Cl⁻
(CH3)2N
C
N(CH3)2

Amino Acid

tryptophan


H
N
CH2CH(NH2)COOH

Benzene

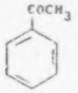


Carbamate derivatives

$R_1NHCOOR_2$

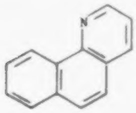
Carbonyl compounds

acetophenone

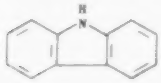


N-Heterocyclics

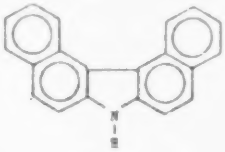
benzo[f]quinoline



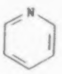
9H carbazole



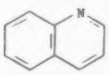
7-H dibenzocarbazole



pyridine

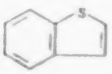


quinoline

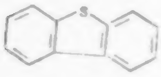


S-Heterocyclics

benzo[b]thiophene

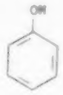


dibenzothiophene



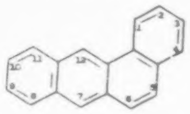
Phenols

phenol

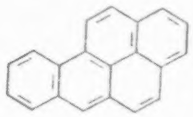


Polynuclear aromatics

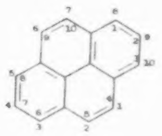
benz[a]anthracene



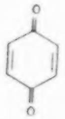
benz[a]pyrene



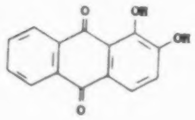
pyrene



Quinone

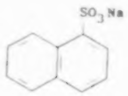


alizarin



Sulfonate

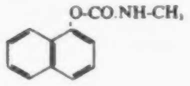
sodium napthalenesulfonate



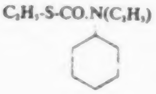
PESTICIDES

Carbamates

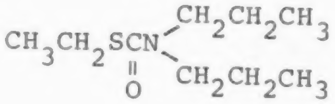
carbaryl



cycloate

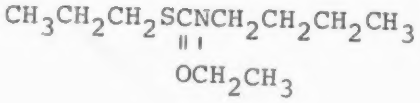

C₂H₅-S-CO.N(C₂H₅)

EPTC



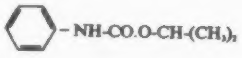
$CH_3CH_2S\underset{\underset{O}{\|}}{C}N\begin{matrix}CH_2CH_2CH_3\\CH_2CH_2CH_3\end{matrix}$

pebulate



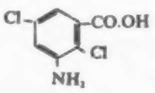
$CH_3CH_2CH_2S\underset{\underset{O}{\|}}{C}\underset{\underset{CH_2CH_3}{|}}{N}CH_2CH_2CH_2CH_3$

propham

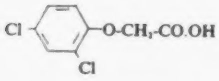

NH-CO.O-CH-(CH₃)₂

Carboxylic Acids

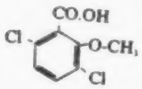
chloramben


Cl
CO.OH
Cl
NH₂

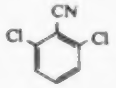
2,4-D


Cl
O-CH₂-CO.OH
Cl

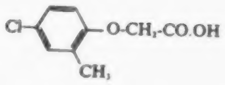
dicamba


CO.OH
Cl
O-CH₃
Cl

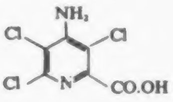
dichlobenil



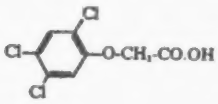
MCPA


Cl
O-CH₂-CO.OH
CH₃

picloram

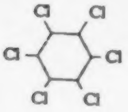

NH₂
Cl
Cl
Cl
N
CO.OH

2,4,5-T

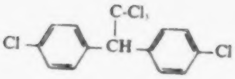

Cl
Cl
O-CH₂-CO.OH
Cl

Halogenated Hydrocarbons

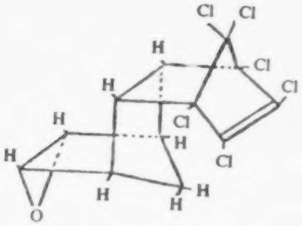
BHC



DDT



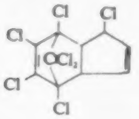
dieldrin



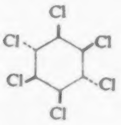
ethylene dibromide

$BrCH_2CH_2Br$

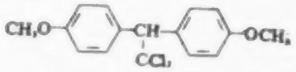
heptachlor



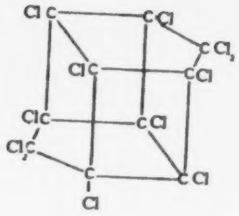
lindane



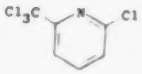
methoxychlor



mirex

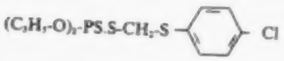


n-serve

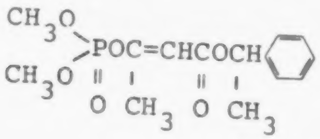


Organophosphates

carbophenothion

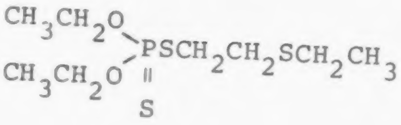


crotoxyphos



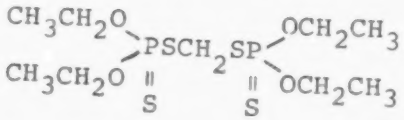
$$\begin{matrix}\mathrm{CH_3O}\\ \mathrm{CH_3O}\end{matrix}\!\gt\!\underset{\underset{\displaystyle \mathrm{O}}{\|}}{\mathrm{P}}\mathrm{O}\underset{\underset{\displaystyle \mathrm{CH_3}}{|}}{\mathrm{C}}\mathrm{{=}CH}\underset{\underset{\displaystyle \mathrm{O}}{\|}}{\mathrm{C}}\mathrm{O}\underset{\underset{\displaystyle \mathrm{CH_3}}{|}}{\mathrm{CH}}$$

disulfoton



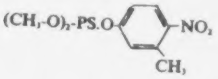
$$\begin{matrix}\mathrm{CH_3CH_2O}\\ \mathrm{CH_3CH_2O}\end{matrix}\!\gt\!\underset{\underset{\displaystyle \mathrm{S}}{\|}}{\mathrm{P}}\mathrm{SCH_2CH_2SCH_2CH_3}$$

ethion

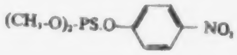


$$\begin{matrix}\mathrm{CH_3CH_2O}\\ \mathrm{CH_3CH_2O}\end{matrix}\!\gt\!\underset{\underset{\displaystyle \mathrm{S}}{\|}}{\mathrm{P}}\mathrm{SCH_2S}\underset{\underset{\displaystyle \mathrm{S}}{\|}}{\mathrm{P}}\!\lt\!\begin{matrix}\mathrm{OCH_2CH_3}\\ \mathrm{OCH_2CH_3}\end{matrix}$$

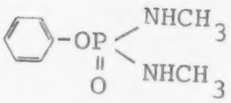
fenitrothion



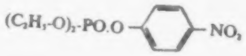
methyl parathion



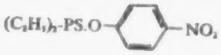
nellite



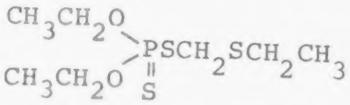
paraoxon



parathion



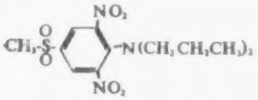
phorate



$$\begin{matrix}CH_3CH_2O\\ CH_3CH_2O\end{matrix}\!>\!\underset{\overset{\|}{S}}{P}SCH_2SCH_2CH_3$$

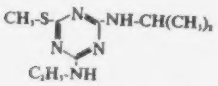
Amino, Nitrophenyl Sulfones

Nitralin

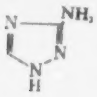


S-Triazines

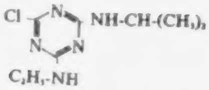
ametryne



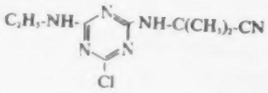
amitrole



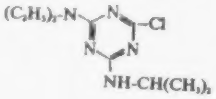
atrazine



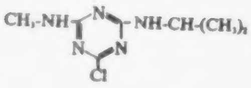
cyanazine



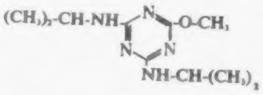
ipazine



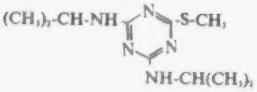
norazine



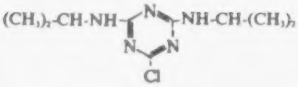
prometone



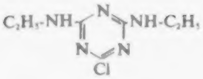
prometryne


(CH3)2-CH-NH
N
S-CH3
N
N
NH-CH(CH3)2

propazine

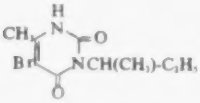

(CH3)2-CH-NH
N
NH-CH-(CH3)2
N
N
Cl

simazine

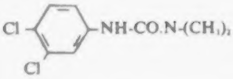

C2H5-NH
N
NH-C2H5
N
N
Cl

Ureas & Uracils

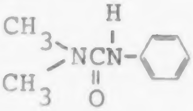
bromacil


H
N
CH3
O
Br
NCH(CH3)-C2H5
O

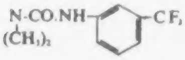
diuron


Cl
NH-CO.N-(CH3)2
Cl

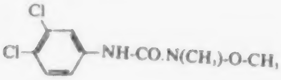
fenuron


CH3
NCN-
H
CH3
O

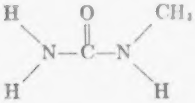
fluometuron


N-CO.NH
(CH3)2
CF3

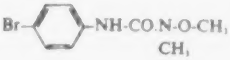
linuron


Cl
Cl
NH-CO.N(CH3)-O-CH3

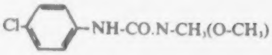
methylurea


H
O
CH3
N
C
N
H
H

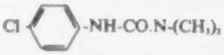
metrobromuron


Br
NH-CO.N-O-CH3
CH3

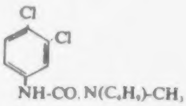
monolinuron


Cl
NH-CO.N-CH3(O-CH3)

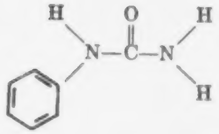
monuron


Cl
NH-CO.N-(CH3)2

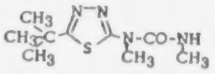
neburon


Cl
Cl
NH-CO. N(C4H9)-CH3

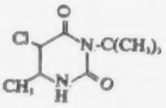
phenylurea



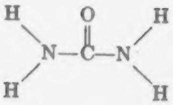
tebuthiuron


CH3
CH3-C
CH3
N—N
S
N-CO-NH
CH3
CH3

terbacil

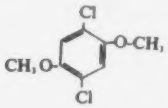

O
Cl
N-C(CH3)3
CH3
N
H
O

urea

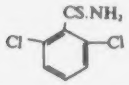


Miscellaneous

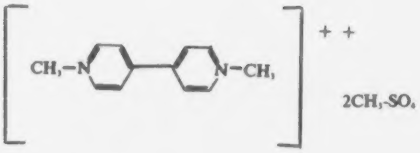
chloroneb


Cl
O-CH3
CH3O
Cl

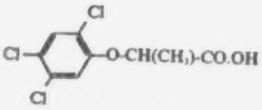
chlorthiamid



paraquat


CH3—N
N—CH3
+ +
2CH3-SO4

silvex


Cl
Cl
O-CH(CH3)-CO.OH
Cl

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